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(54) Title: CRYSTAL STRUCTURE OF ENZYME AND USES THEREOF

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-1-CRYSTAL STRUCTURE OF ENZYME AND USES THEREOF

Field of the Invention

This invention relates to crystallised Aurora A kinase and the use of its threedimensional structure to investigate Aurora kinase homologues and to design Aurora kinase modulators

Background of the Invention

Proteins such as enzymes involved in physiological and pathological processes are important targets in the development of pharmaceutical compounds and treatments.

Knowledge of the three dimensional (tertiary) structure of proteins allows the rational design of mimics or modulators of such proteins. By searching structural databases using structural parameters derived from the protein of interest, it is possible to select molecular structures that may mimic or interact with these parameters. It is then possible to synthesise the selected molecular structure and test its activity. Alternatively, the structural parameters derived from the protein of interest may be used to design and synthesise a mimic or modulator with the desired activity. Such mimics or modulators may be useful as therapeutic agents for treating certain diseases. For example, WO98/07835 discloses crystal structures of a protein tyrosine kinase optionally complexed with one or more compounds. The atomic coordinates of the enzyme structures and any of the bound compounds are used to determine the three-dimensional structures of kinases with unknown structure and to identify modulators of kinase functions. As another example, WO99/01476 discloses the crystal structures of anti-Factor IX. Fab fragments (antibodies) and their use to identify and design new anticoagulant agents.

Knowledge of the three-dimensional structure of a protein is essential for the rational
design of mimics or modulators of that protein. Lack of structural knowledge is a barrier to
the development of new mimics or modulators that may have extremely useful pharmaceutical
properties.

In Eukaryotes, the cell cycle is largely controlled by an ordered cascade of protein phosphorylation. Several families of protein kinases that play critical roles in this cascade have now been identified. The activity of many of these kinases is increased in human tumours when compared to normal tissue. This can occur by either increased levels of expression of the protein (as a result of gene amplification for example), or by changes in expression of co-activators or inhibitory proteins.

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The first identified, and most widely studied of these cell cycle regulators have been the cyclin-dependent kinases (or CDKs). Activity of specific CDKs at specific times is essential for both initiation and coordinated progress through the cell cycle. For example, the CDK4 protein appears to control entry into the cell cycle (the G0-G1-S transition) by 5 phosphorylating the retinoblastoma gene product pRb. This stimulates the release of the transcription factor E2F from pRb, which then acts to increase the transcription of genes necessary for entry into S phase. The catalytic activity of CDK4 is stimulated by binding to a partner protein, Cyclin D1. One of the first demonstrations of a direct link between cancer and the cell cycle was made with the observation that the Cyclin D1 gene was amplified and cyclin 10 D1 protein levels increased (and hence the activity of CDK4 increased) in many human tumours (Reviewed in Sherr, 1996, Science 274: 1672-1677; Pines, 1995, Seminars in Cancer Biology 6: 63-72). Other studies have shown that negative regulators of CDK function are frequently down-regulated or deleted in human tumours, again leading to inappropriate activation of these kinases (Loda et al., 1997, Nature Medicine 3(2): 231-234; Gemma et al., 15 1996, International Journal of Cancer 68(5): 605-11; Elledge et al. 1996, Trends in Cell Biology 6; 388-392).

More recently, protein kinases that are structurally distinct from the CDK family have been identified which play critical roles in regulating the cell cycle and which also appear to be important in oncogenesis. These include the newly-identified human homologues of the 20 Drosophila Aurora and S. cerevisiae Ipl1 proteins. Drosophila Aurora and S. cerevisiae Ipl1, which are highly homologous at the amino acid sequence level, encode serine/threonine protein kinases. Both Aurora and Ipl1 are known to be involved in controlling the transition from the G2 phase of the cell cycle through mitosis, centrosome function, formation of a mitotic spindle and proper chromosome separation / segregation into daughter cells. The three 25 human homologues of these genes, termed Aurora A, B and C, encode cell cycle regulated protein kinases. These show a peak of expression and kinase activity at the G2/M boundary (Aurora A, C) and in mitosis and cytokinesis (Aurora B). Several observations implicate the involvement of human Aurora proteins, in particular Aurora A in cancer. The Aurora A gene maps to chromosome 20q13, a region that is frequently amplified in human tumours including 30 both breast and colon tumours. Aurora A may be the major target gene of this amplicon, since Aurora A DNA is amplified and Aurora A mRNA over expressed in greater than 50% of primary human colorectal cancers. In these tumours Aurora A protein levels appear greatly elevated compared to adjacent normal tissue. In addition, transfection of rodent fibroblasts

-3-

with human Aurora A leads to transformation, conferring the ability to grow in soft agar and form tumours in nude mice (Bischoff et al., 1998, The EMBO Journal. 117(11): 3052-3065).

Other work has shown that artificial over expression of Aurora A leads to an increase in centrosome number and an increase in aneuploidy (Zhou et al., 1998, Nature Genetics. 20(2): 5 189-93).

Importantly, it has also been demonstrated that abrogation of Aurora A expression and function by antisense oligonucleotide treatment of human tumour cell lines (Bischoff and Ploughman, 1999, Trends in Cell Biology, 9(11): 454-459 or by a small molecule inhibitor of Aurora A kinase activity (Keen et al. 2001, poster #2455, American Association for Cancer Research annual meeting, New Orleans USA) leads to defects in mitosis, cell cycle arrest and exerts an antiproliferative effect in these tumour cell lines. This indicates that inhibition of the function of Aurora A will have an antiproliferative effect that may be useful in the treatment of human tumours and other hyperproliferative diseases.

In order to design inhibitors of Aurora A kinase, it is necessary to know the threedimensional structure of Aurora A kinase, in complex with various lead compounds. To date,
the three-dimensional structure of Aurora A kinase has not been available. Further, it has not
been possible to obtain crystals of any part of Aurora of sufficient quality to allow
determination of the structure of the kinase domain including the site of inhibition.

20 Summary of the Invention

The present invention relates to the previously unknown three-dimensional structure of human Aurora A kinase. As described herein, the Applicants have overcome the difficulties encountered by others and have produced crystals of the Aurora A kinase catalytic domain that are of sufficient quality to determine the three-dimensional structure of the protein by X-ray diffraction methods. In addition, the Applicants have determined the three-dimensional crystal structure of the kinase catalytic domain of Aurora A kinase in a complex with the ATP analogue AMP-PNP, as well as the three-dimensional crystal structure of the Aurora A kinase catalytic domain in complex with a synthetic inhibitor. There is a clear need for this structural information to enable identification and structure-based design of new Aurora kinase modulators (particularly inhibitors) for the treatment of various diseases or conditions and in particular diseases of cell proliferation such as cancer. The methods described herein allow the

determination of the three-dimensional structures of Aurora A kinase, as well as other Aurora

kinases, in complex with numerous inhibitors of interest to aid in the rational design of modulators that will treat diseases of cell proliferation.

Brief Description of the Drawings

Figure 1 is a schematic representation of the structure of the [T287D] Aurora A 5 complex with AMP-PNP. The inhibitor has 2 conformations.

Figure 2a is a schematic representation of the structure of Aurora A in complex with a synthetic inhibitor drawn in approximately the same orientation as Figure 1.

Figure 2b is a schematic representation of Aurora A in complex with a synthetic 10 inhibitor, rotated so as to show the extended inhibitor occupying a long active site binding pocket.

Figure 3 is a graph of the activity of [T287D] Aurora A as a function of pH.

Detailed Description of the Invention

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This invention relates to crystals of Aurora A kinase and the use of the threedimensional structure to investigate Aurora kinase homologues and to design Aurora kinase modulators (preferably inhibitors). It further relates to crystals of Aurora kinase, particularly Aurora A kinase, or the catalytic portion thereof, complexed or uncomplexed as described, of sufficient quality to determine the three dimensional (tertiary) structure of the polypeptide by 20 X-ray diffraction methods.

According to a first aspect of the invention, the Applicants provide two crystalline forms of a polypeptide comprising the catalytic domain of Aurora A kinase. One crystalline form is obtained when we crystallise [T287D]Aurora A(122-396) in the presence of the ATPanalogue AMP-PNP. The second crystalline form is obtained when we crystallise GSHM-25 [T287D] Aurora A(122-400) in the presence of a synthetic inhibitor. (Amino acid residues in Aurora A are numbered by taking the first amino acid immediately after the initial methionine as amino acid number one). In one embodiment, the first crystalline form has the space group P3₂21. In another embodiment, the first crystalline form has the unit cell dimensions a = b = 86.55, c = 78.34 Å, $\alpha = \beta = 90$ and $\gamma = 120^{\circ}$. In another embodiment, the second crystalline 30 form has space group P21. In another embodiment, the second crystalline form has the unit

-5-

cell dimensions a = 52.6, b = 88.4, c = 67.8 Å, $\alpha = \gamma = 90$ and $\beta = 90.01^\circ$. In another embodiment, these crystalline forms are described by three-dimensional sets of x,y,zcoordinates (Tables 1 and 2) for each atom in the complex representing the unique repeating motif in the crystal. Table 1 contains the coordinates for the complex molecule in the first 5 crystalline form: Table 2 contains the coordinates for two independent complex molecules in the asymmetric unit (smallest unique repeating unit) in the second crystalline form. In another embodiment, these crystalline forms contain a numerical definition of a binding site, approximated by the set of all residues within a 5 Å contact distance from any atom in either inhibitor. The binding site is defined by the x,y,z-coordinates of atoms in the set of amino acid 10 residues (set A) given by the list Arg136, Leu138, Gly139, Lys140, Gly141, Val146, Ala 159, Lvs161, Leu163, Val177, Glu180, Val181, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215, Thr216, Arg219, Glu259, Asn260, Leu262, Ala272, Asp273, Phe274, Gly275, Trp276, Ser277, Val278, and His279, the atomic coordinates being listed in Tables 1 and 2. The binding site is may be defined in 15 any alternate crystalline form, homologue, variant or mutant wherein the binding site has a root mean square deviation from all atoms of the amino acid residues of not more than 1.0 Å from a least-flexible subset (set B) of the binding site that includes the amino acid residues Arg136, Leu138, Gly139, Val146, Ala159, Lys161, Leu163, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215, Thr216, Arg219, 20 Glu259, Asn260 and Leu262, each having coordinates as described in Tables 1 and 2.

In another embodiment, the first crystalline form comprises a binding site defined by amino acid residues Leu138, Gly139, Val146, Lys161, Val177, Arg178, Arg179, Glu180, Val181, Glu182, Ile183, Gln184, Leu193, Leu209, Tyr211, Ala212, Gly215, Thr216, Glu259, Asn260, Leu262, Ala272, Asp273, Phe274, Gly275, Trp276, Ser277, Val278 and His 279, each having the coordinated listed in Table 1a. An alternative crystalline form, homologue, variant or mutant wherein the binding site has a root mean square deviation from the backbone atoms of the amino acid residues of not more than 1.5 Å, and preferably not more than 1.0 Å is also provided.

In another embodiment, the crystalline forms additionally comprise Aurora kinase
inhibitors in complex with the catalytic domain of Aurora kinase including any of the above
embodiments of the crystalline form.

-6

Another aspect of the invention relates to a method of designing an Aurora chemical modulator using the atomic coordinates of a crystalline form according to any of the above embodiments.

Another aspect of the invention relates to a method of selecting an Aurora chemical modulator using the atomic coordinates of a crystalline form according to any of the above embodiments.

Another aspect of the invention relates to a method of designing or selecting an Aurora chemical modulator using the atomic coordinates of any other protein, e.g. PKA, which has been shown by this invention to have structural similarity to Aurora.

Another aspect of the invention relates to a method of designing an Aurora protein using the atomic coordinates of a crystalline form according to any of the above embodiments.

Another aspect of the invention relates to a method of designing or selecting an Aurora modulator comprising the steps of:

exploring the atomic coordinates of Aurora (Tables 1 and 2) for information on the three-dimensional characteristics of the protein surface;

arriving at an alternative overlapping or non-overlapping binding pocket to the active site ATP binding pocket; and

selecting or designing an Aurora modulator using the binding pocket information.

Another aspect of the invention relates to a method of determining the three-

- 20 dimensional structure of a crystal form of Aurora kinase, referred to as a second or new crystal or crystal form of Aurora kinase, comprising the step of applying difference Fourier or molecular replacement methods using the atomic coordinates of an original crystal of Aurora kinase (from Table 1 or 2) to model the structure of a new crystal, wherein the active site ATP binding pocket of the new crystal is equivalent to that in the first crystal. In a specific
- 25 embodiment, the invention is a method of determining the three-dimensional structure of a crystal form of Aurora kinase A comprising the step of applying difference Fourier or molecular replacement methods using the atomic coordinates of an original (first) crystal of Aurora kinases (from Table 1 or 2) to model the structure of a new crystal or new crystal form of Aurora kinase A, wherein the active site ATP binding pocket of the new crystal is
 30 equivalent to that in the original (first) crystal.

In particular provided herein are crystalline forms of a polypeptide including the catalytic domain of an Aurora A protein. The catalytic domain may be found within the complete protein or within a fragment of the protein. The catalytic domain may be also

-7-

derived from a wild-type Aurora A enzyme or from an Aurora A mutant, homologue or variant. A mutant is a wild type Aurora A protein having one or more changes in its amino acid sequence. An Aurora mutant may have the same activity as the wild type protein, may have modified activity or may be inactive. A variant is a wild type or mutant protein having one or more portions of its sequence removed, or an additional sequence or sequences added, so that the variant is a different length from the wild type or mutant protein. A variant usually has the same activity as the original wild type or mutant protein. A homologue is a related protein in which some parts of the amino acid sequence are the same as in the original protein. Aurora B and Aurora C, for example, are homologues of Aurora A.

The invention relates to crystals of sufficient quality to determine the three dimensional structure to high resolution of any portion, mutant, variant or homologue of Aurora A involving the catalytic domain.

According to a further aspect of the invention, we provide crystalline forms of a
polypeptide containing the Aurora A catalytic domain in complex with small molecular
weight inhibitor molecules. For example, the inhibitor molecule might be a non-hydrolysable
analogue of ATP. Such analogues include, for example, formula I (AMP-PNP). As another
example, the inhibitor might be a molecule synthesised chemically. Such molecules include,
for example, formula II.

Formula I: AMP-PNP

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Formula II

Another aspect of the invention is the unique shape of the active site ATP binding pocket in Aurora. Using X-ray crystallography, we have determined the three-dimensional molecular structure of an Aurora A catalytic domain. Resulting from this, we have determined the unique shape of an Aurora A active site ATP binding pocket (defined by the atomic coordinates of its constituent amino acids). Furthermore, we have determined the spatial arrangement of an Aurora A substrate analogue and an inhibitor molecule relative to the Aurora A active site binding pocket. This structural information can be stored on a computer-readable medium and may be used for rational drug design.

One of the difficulties in studying kinases in general is obtaining active protein. In order to be activated, certain kinases need to be phosphorylated at one or more key amino acid residues. It may be experimentally difficult to obtain 100% pure phosphorylated protein. Different phosphorylation states may have different conformations. Those in the art realise 15 that such heterogeneities in the protein sample can severely impede the ability to form large well-ordered crystals. In Aurora A, phosphorylation of Thr 287 is necessary for activation of the kinase. Replacement of Thr-287 by Asp (an Aurora A mutant called [T287D] Aurora A) provides a mimic of the active protein which can be provided as a homogeneous sample. The [T287D]Aurora A mutant is constitutively active. Thus, preparation of this mutant 20 conveniently addresses both issues of activity and crystallisability.

One of the major hurdles in the crystallisation of multidomain proteins is their
flexibility. To increase the chances of crystallising Aurora A, an enzyme construct limited to
the catalytic domain was used. This provided a more rigid and compact domain. Catalytic
domain constructs can be designed by comparing the amino acid sequence to other kinases of
known structure, and defining start and end residues for the polypeptide encompassing the

.

Aurora A catalytic domain by analogy. This gives numerous possible construct variants, which include the catalytic domain. In order to increase further the chances of crystallising Aurora A, experimental evidence was sought as to which catalytic domain construct would be the most compact while retaining integrity as a folding unit. Limited proteolysis was carried out using endoproteinase Glu-C from Staphylococcus aureus V8 on the catalytic domain. This defined the catalytic domain boundaries to be within residues 122 to 396. Other similar constructs may be obtained through similar procedures, using, for example, different proteases for the limited proteolysis experiment. Such a procedure is exemplified by our preparation, crystallisation and determination of the structure of two Aurora A catalytic domain polypeptides. The structure of [T287D]Aurora A(122-396) in complex with the nonhydrolysable ATP analogue AMP-PNP is shown in Fig. 1. The structure of GSHM-[T287D]Aurora A(122-400) in complex with the synthetic Aurora inhibitor of formula II is shown in Fig. 2a and 2b.

The AMP-PNP molecule occupies a cleft between the N-terminal domain (residues 125 to 208) and the C-terminal domain (residues 215 to 374). Comparison with other kinases demonstrates that this cleft represents a portion of the ATP binding site. Therefore, we have identified the active site ATP binding pocket of Aurora. The electron density shows evidence for the AMP-PNP adopting a dual conformation. In both conformations, the adenine ring and ribose moiety occupy similar pockets with the adenine nitrogen atoms N1 and N6 making classical interactions with main chain atoms in the hinge region (residues 209 to 214) of the enzyme. N1 forms a hydrogen bond with the main chain nitrogen of Ala-212 while N6 forms a hydrogen bond to the peptide carbonyl group of Glu-210. However, torsion angle differences elsewhere in the molecule allow the alpha and beta phosphate groups to occupy alternative pockets. No electron density is apparent in either conformation for the gamma phosphate group of the AMP-PNP molecule. In conformation 1, the beta phosphate group makes polar interactions with the O oxygen atoms of Ser 277 and the side-chain of Asn260, while in conformation 2, the beta phosphate makes polar interactions with the amide carbonyl of -Glu-259 and with a water molecule (Wat-542 in this structure).

From the three-dimensional structure that we have determined for [T287D] Aurora A,
we establish that the AMP-PNP binding pocket, which is the active site ATP binding pocket,
is uniquely defined by the atomic co-ordinates of its constituent amino acid residues, the
coordinates being listed in Tables 1 and 2. An equivalent ATP binding pocket may also be
defined having the same co-ordinates as detailed in Table 1 and with the same constituent

-10-

amino acid residues except that Lys140 and Gly141 in Table 1 and replaced with Ala140 and Ala141, whereby such a table is referred to hereonin as Table 1a.

-11Table 1: coordinates of [T287D] Aurora A (122-396) in complex with AMP-PNP

```
REMARK coordinates from restrained individual B-factor refinement
    REMARK refinement resolution: 500 - 2.2 A
 5 REMARK starting r= 0.2325 free_r= 0.2841
    REMARK final
                       r= 0.2317 free_r= 0.2832
    REMARK B rmsd for bonded mainchain atoms= 1.663 target= 1.5
    REMARK B rmsd for bonded sidechain atoms= 2.408 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.759 target= 2.0
10 REMARK B rmsd for angle sidechain atoms= 3.575 target= 2.5
    REMARK wa= 2.95383
    REMARK rweight=9.122374E-02
    REMARK target= mlf steps= 40
    REMARK sq=P3(2)21 a=86.551 b=86.551 c=78.337 alpha=90 beta=90 gamma=120
15 REMARK parameter file 1 : MSI_CNX_TOPPAR:protein_rep.param
    REMARK parameter file 2 : anp.par
REMARK parameter file 3 : fra.par
    REMARK parameter file 4 : MSI_CNX_TOPPAR:water_rep.param
REMARK parameter file 5 : gly.par
20 REMARK molecular structure file: generate.mtf
    REMARK input coordinates: minimize.pdb
    REMARK reflection file= aurora-dl.cv
    REMARK ness none
    REMARK B-correction resolution: 6.0 - 2.2
25 REMARK initial B-factor correction applied to fobs :
    REMARK B11= -2.797 B22= -2.797 B33= 5.593
REMARK B12= -2.312 B13= 0.000 B23= 0.000
    REMARK B-factor correction applied to coordinate array B: 0.127
    REMARK bulk solvent: (Mask) density level=0.392672e/A^3,B-factor=81.6283 A^2
30 REMARK reflections with | Fobs | /sigma_F < 0.0 rejected REMARK reflections with | Fobs | > 1000 * rms(Fobs) rejected
    REMARK theoretical total number of refl. in resol. range: 17604 (100.0%)
    REMARK number of unobserved reflections (no entry or |F|=0): 841 (4.8%)
                                                                                0.0 %)
    REMARK number of reflections rejected:
                                                                         0 (
                                                                       16763 ( 95.2 %
35 REMARK total number of reflections used:
    REMARK number of reflections in working set:
                                                                        15942 ( 90.6 % )
    REMARK number of reflections in test set:
                                                                          821 (
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42.542 58.531 15.272 1.00 77.20
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6 N GLN A 126
    ATOM
    ATOM
               7 CA GLN A 126
               8 CB GLN A 126
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    ATOM
                 9 CG GLN A 126
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42.092 58.098 18.238 1.00 80.18
41.372 59.925 19.328 1.00 78.24
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40.402 57.676 16.121 1.00 70.19
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50 ATOM
               11 OE1 GLN A 126
12 NE2 GLN A 126
    MOTE
    MOTE
    MOTA
              13 C GLN A 126
              14 O GLN A 126
15 N TRP A 127
16 CA TRP A 127
17 CB TRP A 127
18 CG TRP A 127
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    ATCM:
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                                                                        1.00 69.28
60 ATOM
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               21 CE3 TRP A 127
22 CD1 TRP A 127
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    A TOM
65 ATOM
               25 CZ3 TRP A 127
                26 CH2 TRP A 127
    ATOM
               27 C TRP A 127
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    MOTA
              28 O TRP A 127 39.034 56.724 14.001 1.00 62.11 A
29 N ALA A 128 38.836 54.712 14.975 1.00 57.60 A
30 CA ALA A 128 38.491 54.016 13.740 1.00 52.69 A
                                                                                         А
    MOTA
    MOTA
70 ATOM
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	MOTA	32	C	ALA			37.597	52.820	14.075	1.00 50.40	A	C
	MOTA	33	0	ALA			37.565	52.372	15.220	1.00 48.81	A	O
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3	ATOM	36	CB	LEU			35.235	50.836	11.991	1.00 46.25	A	č
	ATOM	37	CG	LEU			34.125	49.775	12.047	1.00 47.39	A	C
	ATOM	38		LEU			33.068	50.164	13.079	1.00 45.16	A	C
10	ATOM	39	CD2	LEU			33.488	49.630	10.671	1.00 48.56	A	C
10	ATOM	40 41	C	LEU			36.706 36.170	49.936 49.199	13.815 14.645	1.00 48.62 1.00 46.32	A	C
	ATOM	42	N	ALA			37.930	49.724	13.333	1.00 49.46	Ã	N
	ATOM	43	CA	ALA			38.750	48.584	13.742	1.00 50.75	A	Ċ
	ATOM	44	CB	ALA			40.037	48.538	12.907	1.00 50.42	A	C
15	MOTA	45	С	ALA			39.098	48.610	15.233	1.00 51.11	A	C
	MOTA	46	0	ALA			39.559	47.611	15.782	1.00 51.23	A	0
	MOTA	47 48	N CA			131 131	38.896 39.183	49.752	15.883 17.310	1.00 51.02 1.00 51.74	A	C M
	ATOM	49	CB			131	39.353	51.328	17.735	1.00 55.51	A	č
20	ATOM	50	CG			131	40.539	52.012	17.080	1.00 57.37	A	С
	ATOM	51	OD1			131	40.515	52.230	15.852	1.00 60.16	A	0
	ATOM	52	OD2			131	41.496	52.344	17.804	1.00 60.43	A	0
	ATOM	53 54	C	ASP ASP		131	38.041 38.147	49.282 49.195	18.134 19.352	1.00 50.19	A A	C
25	MOTA	55	N			132	36.956	48.881	17.474	1.00 48.84	A	N
20	ATOM	56	CA			132	35.779	48.370	18.181	1.00 47.79	A	č
	ATOM	57	CB			132	34.600	49.327	17.969	1.00 47.00	A	C
	MOTA	58	CG			132	34.877	50.743	18.370	1.00 45.30	A	С
30	MOTA	59				132	34.853 35.148	51.119	19.711 17.404	1.00 45.44	A A	C
50	MOTA	60 61				132 132	35.148	51.708 52.443	20.087	1.00 43.30	A	c
	ATOM	62	CE2			132	35.390	53.034	17.772	1.00 43.84	A	č
	ATOM	63	CZ			132	35.361	53.399	19.115	1.00 42.35	A	c
	MOTA	64	С			132	35.278	46.982	17.801	1.00 48.37	A	C
35	ATOM	65	0			132	35.501	46.505	16.689	1.00 49.60 1.00 47.46	A	O
	ATOM	66 67	N CA	GLU			34.575 33.951	46.350 45.053	18.740 18.501	1.00 47.46	A	C
	ATOM	68	CB	GLU			34.214	44.082	19.661	1.00 48.04	A	C
	MOTA	69	CG	GLU			34.835	42.759	19.214	1.00 49.09	A	C
40	ATOM	70	CD	GLU			34.935	41.725	20.325	1.00 49.60	A	C
	ATOM	71		GLU			33.892	41.172	20.745	1.00 49.55 1.00 49.86	A	0
	ATOM ATOM	72 73	OE2	GLU			36.064 32.460	41.464 45.384	18.418	1.00 49.86	A	0
	ATOM	74	ŏ			133	31.932	46.080	19.282	1.00 41.15	A	ŏ
45	ATOM	75	N	ILE			31.785	44.899	17.380	1.00 44.52	A	N
	ATOM	76	CA	ILE			30.364	45.180	17.194	1.00 44.87	A	C
	ATOM	77	CB	ILE			30.033	45.362 45.739	15.700	1.00 43.36	A	C
	ATOM	78 79	CG2			134	28.567 30.968	46.409	15.540 15.080	1.00 44.27 1.00 45.76	A A	c
50	ATOM	80	CD1	ILE			30.975	47.777	15.776	1.00 43.59	A	c
	ATOM	81	c	ILE			29.420	44.119	17.759	1.00 45.96	A	C
	ATOM	82	0	ILE			29.603	42.927	17.514	1.00 46.32	A	0
	ATOM	83 84	N CA	GLY			28.396	44.571	18.487 19.083	1.00 44.99 1.00 45.95	A A	N
55	MOTA	85	CA	GLY			27.425 26.050	43.661 43.706	18.438	1.00 45.95	A	č
55	ATOM	86	ŏ	GLY			25.918	44.096	17.281	1.00 45.37	A	ŏ
	MOTA	87	N	ARG	А	136	25.014	43.330	19.183	1.00 46.84	A	N
	MOTA	88	CA	ARG			23.652	43.314	18.630	1.00 47.11	A	С
	ATOM	89	CB	ARG			22.665	42.699	19.629	1.00 47.09	A	c
60	MOTA MOTA	90 91	CD	ARG			22.462 21.296	43.505 42.979	20.909 21.736	1.00 45.16 1.00 41.59	A	c
	ATOM	92	NE	ARG			21.296	43.550	23.080	1.00 41.35	A	N
	MOTA	93	CZ	ARG			20.457	44.490	23.507	1.00 41.75	A	C
	ATOM	94		ARG			19.527	44.978	22.701	1.00 41.10	A	N
65	ATOM	95		ARG			20.553	44.949	24.745	1.00 41.12	A	N
	ATOM	96 97	C	ARG			23.116	44.680 45.710	18.205 18.770	1.00 47.41 1.00 46.21	A A	c
	ATOM	98	N	PRO			22.231	44.696	17.197	1.00 49.21	A	N
	ATOM	99	CD	PRO			21.994	43.557	16.295	1.00 50.53	A	C
70	ATOM	100	CA	PRO	Α	137	21.607	45.910	16.659	1.00 50.22	A	C
	ATOM	101	CB	PRO			20.948	45.420	15.373	1.00 49.86	A	C
	ATOM	102	CG	PRO	А	137	21.781	44.245	14.978	1.00 49.74	A	С

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	MOTA	103	С	PRO A	127	20.580	-13- 46.507	17.620	1.00 51.56	A	С
	ATOM	104	ò	PRO A		19.619	45.841	18.007	1.00 52.67	A	ŏ
	ATOM	105	N	LEU A	138	20.783	47.760	18.005	1.00 51.44	A	N
	ATOM	106	CA	LEU A	138	19.851	48.430	18.908	1.00 52.81	A	С
5	ATOM	107	CB	TEA Y	138	20.589	49.498 49.087	19.721 21.086	1.00 52.13 1.00 51.35	A	c
	ATOM ATOM	108 109	CG CD1	LEU A		21.156 21.737	47.694	21.033	1.00 54.20	A	č
	ATOM	110		LEU A	138	22.201	50.093	21.516	1.00 50.21	A	c
	ATOM	111	C	LEU A	138	18.710	49.064	18.114	1.00 53.48	A	C
10	ATOM	112	0	LEU A	138	17.604	49.235	18.620	1.00 53.15	A	0
	MOTA	113	N	GLY A		18.990 17.992	49.401 50.015	16.860 16.009	1.00 55.10 1.00 55.12	A A	N C
	MOTA	114 115	CY	GLY A	139	18.494	50.015	14.586	1.00 57.30	A	č
	ATOM	116	ŏ	GLY A		19.684	50.365	14.348	1.00 55.60	A	ō
15	ATOM	117	N	LYS A	140	17.585	49.930	13.636	1.00 57.79	A	N
	MOTA	118	CA	LYS A	140	17.920	50.004	12.222	1.00 59.68	A	C
	ATOM	119 120	CB	LYS A	140 140	17.898 16.902	48.612 50.897	11.604 11.534	1.00 60.43 1.00 61.09	A	c
	ATOM	121	0	LYS A	140	15.735	50.910	11.912	1.00 61.00	Ã.	ŏ
20	ATOM	122	N	GLY A	141	17.337	51.648	10.530	1.00 62.18	A	N
	ATOM	123	CA	GLY A	141	16.413	52.525	9.834	1.00 62.70	A	C
	MOTA	124	CB	GLY A	141	15.841	53.534	10.803	1.00 65.14 1.00 62.45	A A	C
	MOTA	125 126	C	GLY A	141 141	17.012 18.188	53.241 53.082	8.640 8.325	1.00 62.45	A	Ö
25	ATOM	127	N	ALA A		16.171	54.048	7.999	1.00 62.55	Ä	N
	ATOM	128	CA	ALA A	142	16.522	54.811	6.806	1.00 61.63	A	C
	ATOM	129	CB	ALA A		15.351	55.713	6.416	1.00 62.21	A	C
	ATOM	130	C	ALA A		17.793 18.502	55.641 55.816	6.903 5.910	1.00 60.80 1.00 59.56	A A	c
30	MOTA	131 132	O N	PHE A		18.502	56.152	8.091	1.00 59.81	A	N
50	ATOM	133	CA		143	19.266	56.986	8.255	1.00 58.87	A	C
	ATOM	134	CB	PHE A	143	18.913	58.170	9.153	1.00 61.93	A	С
	ATOM	135	CG	PHE A		18.150	59.246	8.439	1.00 64.91 1.00 65.80	A	C
35	ATOM ATOM	136 137	CD1	PHE A		18.825 16.759	60.244 59.225	7.739 8.407	1.00 65.80	A	č
33	ATOM	138	CE1			18.125	61.206	7.013	1.00 68.03	A	C
	ATOM	139	CE2		143	16.048	60.182	7.683	1.00 67.18	A	C
	MOTA	140	$^{\rm cz}$	PHE A		16.732	61.173	6.984	1.00 67.45	A	C
40	ATOM	141	C	PHE A		20.514	56.275 56.822	8.755 8.694	1.00 56.62 1.00 56.81	A A	0
40	ATOM ATOM	142 143	N	GLY A		20.343	55.050	9.235	1.00 54.51	A	N
	ATOM	144	CA	GLY A	144	21.472	54.289	9.728	1.00 51.51	A	C
	ATOM	145	C	GLY M		21.046	53.257	10.748	1.00 50.01	A	C
40	ATOM	146	0	GLY A	144	19.864 22.011	52.914 52.763	10.849 11.512	1.00 50.62 1.00 47.13	A	O
45	ATOM	147 148	N CA	ASN A		21.731	51.769	12.535	1.00 43.41	A	Ċ
	ATOM	149	CB	ASN A		22.164	50.372	12.065	1.00 44.40	A	C
	MOTA	150	CG	ASN A	145	21.861	50.117	10.598	1.00 44.65	A	C
~~	MOTA	151		ASN A		22.761	50.118 49.900	9.761	1.00 46.61 1.00 45.75	A A	N
50	MOTA	152 153	C ND2	ASN A	145	20.591	52.127	13.788	1.00 40.16	A	C
	ATOM	154	ŏ	ASN A	145	23.491	52.874	13.722	1.00 38.46	A	О
	ATOM	155	N	VAL A		22.082	51.599	14.927	1.00 36.92	A	N
	ATOM	156	CA	VAL A		22.780	51.818 52.590	16.188 17.221	1.00 35.73 1.00 35.98	A A	C
55	ATOM ATOM	157 158	CB CG1	VAL A		22.737	52.590	18.440	1.00 35.98	A	č
	ATOM	159	CG2			21.353	53.868	16.610	1.00 38.31	A	C
	MOTA	160	C	VAL A		23.082	50.414	16.732	1.00 35.97	A	C
	ATOM	161	0	VAL A		22.224	49.537	16.688	1.00 35.59	A	N
60	MOTA	162	N CA	TYR F		24.296	50.197 48.886	17.231 17.763	1.00 37.55 1.00 37.38	A	C
	MOTA	163 164	CB	TYR A		25.674	48.159	16.854	1.00 39.73	A	C
	ATOM	165	CG	TYR F	147	25.324	48.027	15.388	1.00 41.31	A	C
	ATOM	166	CD1			25.614	49.052	14.484	1.00 43.72	A	c
65	MOTA	167	CE1			25.371 24.773	48.900 46.847	13.119 14.890	1.00 41.58	A	C
	ATOM	168 169	CD2			24.773	46.847	13.534	1.00 42.29	A	c
	ATOM	170	CZ	TYR A	147	24.832	47.712	12.656	1.00 43.10	A	C
	ATOM	171	OH	TYR 7		24.619	47.533	11.312	1.00 43.57	A	0
70	ATOM	172	C	TYR A		25.352	48.972	19.116	1.00 37.06	A	C
	MOTA	173 174	N	TYR A		25.950 25.277	49.985 47.879	19.466 19.864	1.00 36.75 1.00 36.10	A	N
	ATOM	1/4	14	DEC 1	140	43.411	47.079	19.004	1.00 30.10	-	**

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	ATOM	175	CA	LEU			25.970	47.790	21.133		35.79	A	C
	MOTA	176	CB	LEU			25.466	46.574	21.911		38.69	A	С
	ATOM	177	CG	LEU			25.919	46.357	23.350	1.00	41.70	A	C
-	ATOM	178		LEU			25.512	47.550	24.213		44.96	A	C
5	ATOM	179	CD2	LEU			25.285 27.407	45.083 47.562	23.876		41.80	A	c
	ATOM	180 181	0	LEU			27.606	46.984	19.593		35.45	A	0
	ATOM	182	N	ALA		149	28.404	48.033	21.395		36.28	A	N
	ATOM	183	CA	ALA		149	29.791	47.829	20.989		37.35	A	C
10	ATOM	184	CB	ALA			30.211	48.870	19.943		35.81	A	C
	ATOM	185	C	ALA	A	149	30.728	47.894	22.182	1.00	40.30	A	C
	ATOM	186	0	ALA		149	30.341	48.301	23.278	1.00	39.46	A	0
	MOTA	187	N	ARG			31.974	47.498	21.962	1.00	41.71	A	N
	ATOM	188	CA	ARG			32.956	47.506	23.026	1.00	45.19	A	c
15	ATOM	189	CB	ARG			32.946	46.137 45.984	23.717	1.00	49.42 52.01	A	C
	ATOM ATOM	190 191	CD	ARG		150 150	33.892 33.362	44.946	25.885	1.00	54.44	A	č
	ATOM	192	NE	ARG			32.854	43.742	25.231	1.00	55.30	A	N
	ATOM	193	CZ	ARG			32.082	42.837	25.828	1.00	53.68	A	Ċ
20	ATOM	194	NH1	ARG			31.729	42.996	27.095	1.00	54.04	A	N
	ATOM	195		ARG			31.652	41.781	25.154		52.52	A	N
	MOTA	196	C	ARG	A	150	34.322	47.829	22.440		47.01	A	C
	MOTA	197	0	ARG		150	34.703	47.296	21.397		47.88	A	0
0.5	MOTA	198	N	GLU		151	35.042	48.730	23.093	1.00	49.42	A	N
25	MOTA	199 200	CB	GLU		151 151	36.365 36.848	49.124 50.346	22.632 23.426		54.61 56.69	A	č
	MOTA	201	CG		Â	151	37.983	51.140	22.766		63.91	A	č
	ATOM	202	CD			151	39.363	50.535	22.995		66.90	A	č
	ATOM	203	OE1			151	39.845	50.581	24.151	1.00		A	0
30	ATOM	204	OE2	GLU	A	151	39.967	50.018	22.024	1.00	69.20	A	0
	MOTA	205	C		A	151	37.265	47.917	22.871	1.00	56.41	A	C
	ATOM	206	0			151	37.304	47.384	23.975		56.29	A	0
	MOTA	207	N		A	152	37.963	47.471	21.830		59.00	A	N C
35	MOTA	208 209	CA		A	152 152	38.842 39.626	46.305 46.114	21.934	1.00	61.26	A	c
33	ATOM	210	CG		Â	152	38.765	45.794	19.402		61.58	A	č
	ATOM	211	CD		Ä	152	39.643	45.531	18.171		62.51	A	C
	ATOM	212	CE		A	152	38.831	45.211	16.916	1.00	61.68	A	C
	MOTA	213	NZ			152	37.959	44.023	17.075	1.00	63.73	A	N
40	MOTA	214	C			152	39.816	46.390	23.111	1.00	61.70	A	c
	ATOM	215	0		A	152	39.759	45.572	24.030	1.00	60.64	A	0
	MOTA	216	N	GLN		153 153	40.702	47.381 47.562	23.083 24.145	1.00	63.23	A	N
	MOTA	217 218	CB	GLN		153	42.477	48.859	23.916	1.00	68.76	A	č
45	ATOM	219	CG		Â	153	43.247	48.912	22.597	1.00	72.76	A	č
	ATOM	220	CD		Ā	153	44.497	48.038	22.595	1.00	75.69	A	č
	ATOM	221			Ä	153	44.438	46.835	22.872	1.00	75.15	A	0
	ATOM	222	NE2		A	153	45.639	48.644	22.273	1.00	76.04	A	N
	ATOM	223	C		Α	153	41.055	47.600	25.535	1.00	67.63	A	c
50	ATOM	224	0		A		41.276	46.709	26.360	1.00	67.71	A	0
	ATOM	225 226	N CA		A A	154 154	40.265 39.592	48.642 48.858	25.776 27.054	1.00	67.64 68.46	A	N C
	ATOM	227	CB	SER			38.963	50.253	27.054	1.00	68.69	A	č
	ATOM	228	OG	SER			38.180	50.435	28.231	1.00	72.14	A	ŏ
55	ATOM	229	c			154	38.524	47.827	27.413	1.00	67.39	A	C
	ATOM	230	0	SER	A	154	38,422	47.404	28.562	1.00	66.91	A	0
	ATOM	231	N			155	37.722	47.447	26.426	1.00	66.94	A	
	ATOM	232	CA	LYS			36.645	46.479	26.602	1.00	65.83	A	
60	ATOM	233	CB	LYS			37.166	45.229	27.310 26.452	1.00	66.50	A	C
60	ATOM ATOM	234 235	CD	LYS		155	38.159 38.437	44.456	26.432	1.00	70.98	A	č
	ATOM	236	CE	LYS			39.396	42.318	26.080	1.00	72.81	A	
	ATOM	237	NZ			155	39.663	40.936	26.573	1.00		A	
	ATOM	238	C	LYS	A	155	35.422	47.053	27.326	1.00	64.74	A	C
65	ATOM	239	0	LYS	A	155	34.608	46.318	27.891	1.00		A	
	ATOM	240	N	PHE			35.289	48.375	27.278	1.00	63.83	A	
	ATOM	241	CA	PHE			34.162	49.061	27.901	1.00	61.40	A	
	MOTA	242 243	CB	PHE			34.544 33.478	50.514	28.194 28.911	1.00	63.97 68.01	A	
70	ATOM ATOM	244		PHE	*	156	32.956	51.290 50.832	30.121		69.99	A	
70	ATOM	245	CD2	PHE	A	156	33.004	52.490	28.387	1.00	68.86	A	
	ATOM	246		PHE			31.975	51.559	30.800	1.00	70.97	A	

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	ATOM	247	CE2	PHE A 15	6 32.026	53.224	29.055	1.00 69.64	A	C
	MOTA	248	CZ	PHE A 15	6 31.510	52.759	30.264	1.00 70.88	A	C
	MOTA	249	С	PHE A 15		49.013	26.946	1.00 57.88	A	C
_	MOTA	250	0	PHE A 15		49.157	25.732	1.00 55.27	A	N
5	ATOM	251	N	ILE A 15		48.799	27.498 26.701	1.00 53.85	A	C
	ATOM	252	CA	ILE A 15		48.730 47.949	27.459	1.00 50.05	A	č
	ATOM	253 254	CG2	TLE A 15		48.111	26.760	1.00 48.39	A	č
	ATOM	255	CG1			46.464	27.545	1.00 51.64	A	č
10	ATOM	256	CD1			45.707	26.244	1.00 52.26	A	C
	ATOM	257	C	ILE A 15		50.130	26.353	1.00 47.74	A	C
	ATOM	258	0	ILE A 15	7 29.998	51.021	27.203	1.00 45.67	A	0
	ATOM	259	N	LEU A 15		50.308	25.097	1.00 44.24	A	N
	MOTA	260	CA	LEU A 15	8 29.079	51.586	24.618	1.00 43.05	A	C
15	ATOM	261	CB	LEU A 15		52.539 52.029	24.251 23.327	1.00 42.08 1.00 45.57	A A	c
	MOTA	262 263	CG CD1	LEU A 15 LEU A 15		51.994	21.901	1.00 46.09	A	č
	MOTA MOTA	264	CD2			52.940	23.435	1.00 46.27	A	č
	ATOM	265	c	LEU A 15		51.392	23.427	1.00 39.34	A	C
20	ATOM	266	ō	LEU A 15		50.269	23.036	1.00 38.00	A	0
	ATOM	267	N	ALA A 15		52.489	22.858	1.00 39.30	A	N
	MOTA	268	CA	ALA A 15		52.384	21.702	1.00 38.21	A	c
	ATOM	269	CB	ALA A 15		53.007	22.006	1.00 37.68	A A	C
	MOTA	270	C	ALA A 15		53.082 54.073	20.525	1.00 38.81	A	0
25	MOTA	271 272	O	ALA A 15 LEU A 16		52.556	19.329	1.00 39.75	A	N
	ATOM	273	CA	LEU A 16		53.152	18.145	1.00 39.68	A	C
	MOTA	274	CB	LEU A 16		52.175	17.503	1.00 41.87	A	C
	ATOM	275	CG	LEU A 16		52.748	16.543	1.00 44.90	A	C
30	ATOM	276	CD1			53.651	17.305	1.00 43.49	A	C
	MOTA	277	CD2			51.604	15.885	1.00 44.40	A	c
	MOTA	278	C	LEU A 16		53.496	17.169	1.00 39.67 1.00 39.99	A A	C
	ATOM	279 280	O N	LEU A 16 LYS A 16		52.610 54.788	16.666 16.921	1.00 38.00	A	N
35	ATOM ATOM	281	CA	LYS A 16	1 25.461	55.212	15.996	1.00 39.14	A	c
33	MOTA	282	CB	LYS A 16	1 24.782	56.501	16.480	1.00 40.21	A	C
	ATOM	283	CG	LYS A 16	1 23.783	57.073	15.485	1.00 43.91	A	C
	ATOM	284	CD	LYS A 16	1 23.120	58.347	15.994	1.00 45.72	A	C
	ATOM	285	CE	LYS A 16		58.060	17.140	1.00 48.13	A	c
40	ATOM	286	NZ	LYS A 16	1 21.511	59.299 55.429	17.670 14.644	1.00 52.12	A	N C
	ATOM	287	C	LYS A 16		56.294	14.485	1.00 35.11	A	ŏ
	ATOM	288 289	O N	LYS A 16		54.631	13.677	1.00 37.87	A	N
	ATOM	290	CA	VAL A 16		54.656	12.311	1.00 37.92	A	C
45	ATOM	291	CB	VAL A 16		53.201	11.807	1.00 39.41	A	C
	ATOM	292	CG1	VAL A 16	2 27.179	53.214	10.506	1.00 37.99	A	C C
	ATOM	293	CG2			52.382	12.873	1.00 37.26	A	c
	MOTA	294	C	VAL A 16		55.362	11.368	1.00 39.49	A A	0
50	MOTA	295 296	O N	VAL A 16		54.878 56.500	10.817	1.00 39.18	A	N
30	MOTA	297	CA	LEU A 16		57.277	9.907	1.00 42.61	A	c
	ATOM	298	CB	LEU A 16		58.726	10.400	1.00 43.27	A	C
	ATOM	299	CG	LEU A 16	3 23.621	59.124	11.457	1.00 42.79	A	C
	ATOM	300		LEU A 16		57.944	12.311	1.00 43.48	A	C
55	ATOM	301		LEU A 16		60.246	12.313	1.00 43.16	A	c
	ATOM	302	c	LEU A 16		57.278 57.515	8.466 8.228	1.00 45.56	A A	0
	ATOM	303 304	N	LEU A 16		57.029	7.513	1.00 48.16	A	N
	MOTA	305	CA	PHE A 1		57.006	6.091	1.00 52.24	A	Ċ
60	ATOM	306	CB	PHE A 1		56.332	5.286	1.00 53.67	A	C
-	ATOM	307	CG	PHE A 1	4 23.201	55.008	5.831	1.00 55.86	A	C
	ATOM	308		PHE A 1		54.625	5.781	1.00 56.34	A	C
	MOTA	309		2 PHE A 1		54.139	6.392	1.00 55.83	A	C
	ATOM	310	CEI			53.393	6.286	1.00 58.23	A A	C
65	MOTA	311 312	CE	PHE A 1			6.897 6.846	1.00 55.86 1.00 58.79	A	C
	MOTA	313	C	PHE A 1			5.551	1.00 53.31	A	č
	ATOM	314	ŏ	PHE A 1			5.676	1.00 51.66	A	ō
	ATOM	315	N	LYS A 1			4.940	1.00 55.24	A	N
70	MOTA	316	CA	LYS A 1			4.372	1.00 57.91	A	C
	MOTA	317	CB	LYS A 1			3.754	1.00 57.31	A	C
	ATOM	318	CG	LYS A 1	55 28.881	60.126	4.756	1.00 57.21	A	С

							-16-				
	ATOM	319	CD	LYS A		30.201	60.338	4.040	1.00 57.36	A	C
	MOTA	320	CE	LYS A		31.340	60.528	5.018	1.00 58.00	A	C N
	ATOM	321	NZ	LYS A		32.638 25.340	60.675 60.392	4.309	1.00 60.01	A A	C
5	ATOM	322 323	C	LYS A		24.971	61.559	3.194	1.00 59.56	A	ŏ
5	ATOM	324	N	ALA A		24.894	59.407	2.534	1.00 62.03	A	N
	ATOM	325	CA	ALA A		23.931	59.628	1.462	1.00 66.28	A	С
	ATOM	326	CB	ALA A	166	23.673	58.319	0.728	1.00 65.88	A	C
	MOTA	327	C	ALA A		22.606	60.229	1.939	1.00 69.38	A	C
10	MOTA	328	0	ALA A		21.706	60.485	1.132	1.00 69.73	A	O N
	MOTA	329	N	GLN A		22.486 21.272	60.447 61.017	3.246 3.819	1.00 70.89	A A	C
	MOTA	330 331	CA	GLN A		20.686	60.063	4.856	1.00 73.19	A	č
	ATOM	332	CG	GLN A		20.621	58.625	4.388	1.00 76.66	A	č
15	ATOM	333	CD	GLN A		19.769	58.453	3.152	1.00 79.08	A	C
	ATOM	334	OE1			19.772	57.390	2.527	1.00 80.82	A	0
	ATOM	335	NE2	GLN A		19.025	59.497	2.792	1.00 80.53	A	N
	MOTA	336	C	GLN A		21.597	62.352 63.336	4.477	1.00 72.50	A	C
20	MOTA	337 338	N	GLN A		20.884	62.379	5.247	1.00 73.59	A	N
20	MOTA	339	CA	LEU A		23.082	63.602	5.912	1.00 76.12	Ä	c
	MOTA	340	СВ	LEU A		24.460	63.421	6.552	1.00 74.15	A	C
	ATOM	341	CG	LEU A	168	24.547	62.317	7.612	1.00 73.50	A	С
	ATOM	342		LEU A		25.979	62.150	8.066	1.00 72.46	A	C
25	ATOM	343	CD2			23.656	62.665	8.789 4.881	1.00 72.72	A	C
	ATOM	344	C	LEU A		23.112 22.254	64.728 65.610	4.881	1.00 79.50	A	Ö
	ATOM ATOM	345 346	N	GLU 2		24.086	64.681	3.976	1.00 81.12	A	N
	ATOM	347	CA		169	24.228	65.697	2.936	1.00 83.10	A	C
30	MOTA	348	CB	GLU 2		25.344	65.296	1.971	1.00 83.78	A	С
	MOTA	349	CG	GLU Z		25.096	63.979	1.255	1.00 85.16	A	C
	MOTA	350	CD	GLU 2		26.298	63.510	0.457	1.00 86.11	A A	C
	MOTA	351	OE1 OE2	GLU A		27.361 26.179	63.266 63.387	1.068	1.00 85.05 1.00 87.77	A	0
35	ATOM	352 353	C	GLU Z		22.924	65.891	2.164	1.00 83.83	Ä	č
55	ATOM	354	õ	GLU 2		22.541	67.018	1.840	1.00 83.53	A	ō
	ATOM	355	N	LYS 2	170	22.250	64.782	1.878	1.00 84.15	A	N
	ATOM	356	CA	LYS 2		20.985	64.794	1.149	1.00 85.24	A	c
	ATOM	357	CB	LYS I		20.809	63.467	0.411	1.00 84.77	A	c
40	MOTA	358	CG	LYS I		19.407 19.271	63.207 61.764	-0.112 -0.560	1.00 84.91 1.00 84.46	A A	c
	MOTA	359 360	CE	LYS		17.863	61.447	-1.022	1.00 84.75	A	č
	ATOM	361	NZ	LYS		17.754	60.021	-1.434	1.00 84.95	A	N
	ATOM	362	C	LYS 2	170	19.797	65.020	2.085	1.00 86.98	A	С
45	ATOM	363	0	LYS 2		19.175	64.058	2.547	1.00 88.55	A	0
	ATOM	364	N	ALA :		19.495	66.291	2.353	1.00 86.65	A A	N
	ATOM	365 366	CB	ALA A		18.388 17.388	66.702 65.561	3.222	1.00 86.88 1.00 86.71	A	c
	ATOM	367	C	ALA		18.877	67.194	4.577	1.00 86.86	Ä	č
50	ATOM	368	ŏ	ALA		19.133	68.386	4.754	1.00 86.68	A	0
	ATOM	369	N	GLY :		18.993	66.275	5.533	1.00 86.88	A	N
	ATOM	370	CA		172	19.449	66.635	6.866	1.00 86.26	A A	c
	ATOM	371	c		A 172	20.858 21.659	67.190 66.924	6.837 7.735	1.00 86.14 1.00 86.73	A	0
55	MOTA	372 373	N	GLY .		21.141	67.967	5.793	1.00 85.19	A	N
33	MOTA	374	CA	VAL .		22.437	68.593	5.564	1.00 83.10	A	c
	ATOM	375	СВ	VAL		22.280	70.107	5.336	1.00 82.25	A	С
	ATOM	376	CG1			23.622	70.720	4.988	1.00 79.89	A	c
	ATOM	377	CG2			21.276	70.355	4.223	1.00 82.16	A	c
60	ATOM	378	c	VAL .		23.450	68.364 68.599	6.678 7.857	1.00 82.27	A A	0
	ATOM	379 380	N	GLU		24.629	67.897	6.289	1.00 80.75	A	N
	ATOM	381	CA	GLU		25.690	67.639	7.242	1.00 79.61	A	C
	ATOM	382	CB	GLU		26.984	67.310	6.492	1.00 80.39	A	C
65	ATOM	383	CG	GLU .	A 174	28.221	67.233	7.369	1.00 81.70	A	C
	MOTA	384	CD	GLU		28.904	68.577	7.535	1.00 83.27	A	c
	MOTA	385	OE1			29.877 28.474	68.658 69.552	8.314 6.879	1.00 83.32	A A	0
	ATOM	386 387	OE2	GLU		25.886	68.848	8.151	1.00 83.99	A	c
70	ATOM	388	Ö	GLU		26.258	68.701	9.313	1.00 78.22	A	ō
, ,	ATOM	389	N	HIS		25.618	70.038	7.615	1.00 78.24	A	N
	ATOM	390	CA		A 175	25.770	71.285	8.363	1.00 77.47	A	C

							-17-				
	ATOM	391	CB	HIS A		25.205	72.463	7.562	1.00 76.98	A	C
	MOTA	392 393	CG CD2	HIS A		25.859 26.828	72.663 71.962	6.231 5.597	1.00 77.17	A A	c
	ATOM	393		HIS A		25.506	73.687	5.378	1.00 77.46	A	N
5	ATOM	395		HIS A		26.229	73.607	4.275	1.00 77.33	A	c
	ATOM	396	NB2	HIS A		27.039	72.568	4.382	1.00 77.65	A	N
	MOTA	397	C	HIS A	175	25.073	71.223	9.716	1.00 76.86	A	С
	MOTA	398	0	HIS A		25.709	71.382	10.756	1.00 74.77	A	0
	MOTA	399	N	GLN A		23.761	70.998	9.684	1.00 77.67	A	N
10	MOTA	400 401	CA CB	GLN A		22.946 21.495	70.907	10.893	1.00 79.14	A A	C
	MOTA	401	CB	GLN A		20.643	70.583	11.673	1.00 79.88	A	c
	ATOM	403	CD	GLN A		19.203	69.804	11.272	1.00 83.00	A	č
	ATOM	404	OE1	GLN A		18.444	69.197	12.028	1.00 82.78	A	ō
15	MOTA	405	NE2	GLN A	176	18.818	70.257	10.081	1.00 83.25	A	N
	ATOM	406	C	GLN A		23.459	69.858	11.873	1.00 79.66	A	С
	ATOM	407	0	GLN A		23.533	70.103	13.079	1.00 78.29	A	0
	ATOM	408	N	ALA A		23.816 24.305	68.689 67.596	11.348 12.178	1.00 81.28 1.00 82.55	A	C
20	MOTA	409 410	CA	ALA A		23.604	66.305	11.786	1.00 83.52	A	c
20	ATOM	411	C	ALA A		25.814	67.399	12.113	1.00 83.96	A	č
	ATOM	412	ŏ	ALA A		26.284	66.312	11.767	1.00 85.89	A	ō
	ATOM	413	N	ARG A	178	26.575	68.438	12.447	1.00 84.10	A	N
	ATOM	414	CA	ARG A		28.029	68.327	12.426	1.00 84.25	A	C
25	ATOM	415	CB	ARG A		28.612	68.952	11.160	1.00 83.50	A	C
	ATOM	416	CG	ARG A		30.132	69.065	11.216 11.659	1.00 84.36 1.00 83.46	A	C
	MOTA	417 418	CD	ARG A		30.782 32.208	67.748 67.902	11.948	1.00 83.46	A	N
	ATOM	419	CZ	ARG A		32.704	68.564	12.990	1.00 79.87	A	č
30	ATOM	420		ARG A		31.897	69.144	13.867	1.00 78.59	A	N
	MOTA	421	NH2	ARG A	178	34.017	68.652	13.149	1.00 78.59	A	N
	ATOM	422	C	ARG A		28.735	68.923	13.639	1.00 83.89	A	C
	ATOM	423	0	ARG A		29.075	68.199	14.576	1.00 84.19	A	0
35	MOTA	424	N	ALA A		28.971 29.657	70.234 70.913	13.610 14.711	1.00 83.02 1.00 81.63	A A	N
33	MOTA	425 426	CA	ALA A		29.708	72.420	14.457	1.00 82.10	A	č
	ATOM	427	C	ALA A		28.928	70.622	16.010	1.00 80.48	A	č
	ATOM	428	o	ALA A		29.497	70.733	17.102	1.00 79.55	A	0
	ATOM	429	N	GLU A		27.658	70.253	15.869	1.00 79.39	A	N
40	ATOM	430	CA	GLU A	180	26.815	69.908	17.002	1.00 78.29	A	C
	ATOM	431	CB	GLU A		25.389 24.543	69.647 70.903	16.521 16.382	1.00 78.71	A	C
	ATOM	432 433	CD	GLU A		25.322	72.098	15.848	1.00 83.43	A	č
	MOTA	434		GLU A		26.170	72.639	16.591	1.00 84.35	A	ŏ
45	ATOM	435	OE2			25.088	72.499	14.686	1.00 84.07	A	0
	MOTA	436	C	GLU A		27.382	68.681	17.713	1.00 75.99	A	C
	ATOM	437	0	GLU A		26.838	68.226	18.720	1.00 75.11	A	0
	ATOM	438 439	N	VAL A		28.471 29.148	68.146 66.999	17.165 17.757	1.00 73.03 1.00 70.84	A	N
50	ATOM	440	CB	VAL A		29.148	66.175	16.706	1.00 70.79	A	č
50	ATOM	441	CG1			30.861	65.180	17.409	1.00 69.55	A	C
	ATOM	442	CG2			28.973	65.433	15.791	1.00 69.51	A	C
	ATOM	443	C	VAL A	. 181	30.128	67.585	18.758	1.00 69.44	A	C
	ATOM	444	0	VAL A		30.351	67.026	19.831	1.00 69.27	A	0
55	ATOM	445	N	ALA A		30.707	68.724	18.392 19.259	1.00 68.30 1.00 66.45	A	N
	ATOM	446 447	CA	ALA A		31.654 32.419	69.416 70.483	18.469	1.00 67.64	A	c
	ATOM	448	CD	ALA A		30.900	70.057	20.425	1.00 64.52	A	č
	MOTA	449	ŏ	ALA A		31.368	70.013	21.567	1.00 64.11	A	o
60	MOTA	450	N	ILE A	183	29.737	70.649	20.146	1.00 59.92	A	N
	MOTA	451	CA	ILE A		28.969	71.262	21.222	1.00 59.47	A	C
	MOTA	452	CB		183	27.772	72.131	20.710	1.00 60.11	A	C
	MOTA	453	CG2		183	28.277	73.193	19.744	1.00 60.37 1.00 60.21	A	C
65	ATOM	454 455	CD1			26.705 25.391	71.251	19.783	1.00 60.21	A	c
03	ATOM	456	CDI	TLE A		28.437	70.164	22.140	1.00 56.99	A	c
	ATOM	457	ō	ILE A		28.617	70.229	23.350	1.00 56.38	A	0
	ATOM	458	N	GLN A		27.799	69.150	21.562	1.00 56.33	A	N
	ATOM	459	CA	GLN A		27.264	68.045	22.352	1.00 56.17	A	C
70	MOTA	460 461	CB	GLN F		26.552 25.670	67.026 66.045	21.458	1.00 57.52 1.00 61.39	A	C
	ATOM	462	CD	GLN A		24.324	66.650	22.226	1.00 64.82	A	č
	2101	402	-	J 1		24.524	30.030	55.015		.,	-

							-18-				
	ATOM	463	OE1	GLN 2	184	23.672	66.213	23.570	1.00 62.62	A	0
	ATOM	464	NE2	GLN A		23.897	67.654	21.857	1.00 65.33	A	N
	ATOM	465	C	GLN A		28.381	67.342	23.124	1.00 54.27	A	C
_	ATOM	466	0	GLN A		28.236	67.057	24.308	1.00 53.30	A	0
5	ATOM	467 468	N	SER A		29.498	67.076 66.401	22.458 23.106	1.00 53.49 1.00 55.92	A	N
	ATOM	468	CA	SER A		30.621 31.786	66.247	22.128	1.00 56.01	A	c
	ATOM	470	OG	SER A		32.335	67.510	21.797	1.00 55.72	Ä	ő
	ATOM	471	C	SER A		31.115	67.152	24.342	1.00 56.22	A	C
10	ATOM	472	0	SER A		31,636	66.551	25.281	1.00 55.88	A	0
	MOTA	473	N	HIS A		30.945	68.467	24.341	1.00 56.92	A	N
	ATOM	474 475	CA	HIS A	186	31.399 31.765	69.281 70.676	25.460 24.953	1.00 58.35 1.00 61.17	A A	C
	ATOM	476	CG	HIS A		32.936	70.683	24.933	1.00 64.95	A	c
15	ATOM	477		HIS A		33.986	69.834	23.898	1.00 65.77	A	č
	ATOM	478		HIS A		33.120	71.656	23.056	1.00 66.54	A	N
	ATOM	479		HIS A		34.231	71.404	22.386	1.00 66.45	A	C
	ATOM	480		HIS 2		34.775	70.305	22.877	1.00 66.45	A	N
20	ATOM	481 482	C	HIS A		30.399 30.615	69.359 70.079	26.610 27.583	1.00 56.48	A	C
20	ATOM	483	N	LEU 2		29.304	68.614	26.496	1.00 53.92	A	N
	ATOM	484	CA	LEU 2		28.296	68.580	27.543	1.00 52.14	A	c
	ATOM	485	CB	LEU 2	187	26.900	68.410	26.935	1.00 51.03	A	C
	ATOM	486	CG	LEU 2		26.067	69.660	26.626	1.00 52.63	A	C
25	ATOM	487	CD1			26.958	70.858	26.344	1.00 52.17 1.00 51.26	A	C
	ATOM	488 489	CD2 C	PEA 1	187	25.158 28.619	69.365 67.401	25.444 28.454	1.00 51.26	A	c
	ATOM	490	õ	LEU A		28.631	66.256	28.010	1.00 51.83	A	ŏ
	ATOM	491	N		188	28.891	67.682	29.724	1.00 50.85	A	N
30	ATOM	492	CA		188	29.213	66.626	30.676	1.00 49.45	A	C
	MOTA	493	CB		188	30.703	66.670	31.026	1.00 52.24	A	C
	ATOM	494	CG	ARG I		31.595	66.327	29.838	1.00 56.65	A A	C
	ATOM ATOM	495 496	CD	ARG A		33.042 33.881	66.111 65.699	30.252 29.126	1.00 61.31 1.00 64.86	A	N
35	ATOM	497	CZ	ARG		34.195	66.477	28.092	1.00 65.93	A	c
	ATOM	498		ARG		33.744	67.725	28.028	1.00 67.33	A	N
	MOTA	499		ARG :		34.959	66.007	27.115	1.00 66.11	A	N
	ATOM	500	C	ARG		28.356	66.746	31.923	1.00 47.99	A	C
40	ATOM	501 502	N	ARG A		28.619 27.323	67.561 65.913	32.813 31.981	1.00 47.40 1.00 46.41	A A	N
70	ATOM	503	CA	HIS		26.387	65.939	33.095	1.00 43.42	A	ĉ
	ATOM	504	CB	HIS 2	189	25.288	66.961	32.775	1.00 39.93	A	C
	ATOM	505	CG	HIS :	A 189	24.371	67.255	33.918	1.00 37.78	A	C
	ATOM	506		HIS I		24.342	68.289	34.793	1.00 37.18	A	C
45	ATOM	507		HIS		23.322	66.431 66.948	34.261 35.296	1.00 38.04	A	N C
	ATOM	508 509		HIS I		23.281	68.076	35.637	1.00 38.70	A	N
	ATOM	510	C	HIS		25.794	64.546	33.314	1.00 42.45	A	c
	ATOM	511	ō	HIS		25.585	63.799	32.367	1.00 43.83	A	0
50	ATOM	512	N	PRO 2		25.539	64.171	34.576	1.00 41.87	A	N
	ATOM	513	CD	PRO 2		25.811	64.893	35.829	1.00 41.35	A	C
	ATOM	514 515	CB	PRO I		24.970 24.878	62.850 62.820	34.851 36.378	1.00 40.95 1.00 40.22	A A	c
	ATOM	516	CG	PRO		24.803	64.267	36.758	1.00 43.23	A	č
55	ATOM	517	C		A 190	23.626	62.591	34.178	1.00 40.60	A	C
	ATOM	518	0	PRO .		23.260	61.442	33.931	1.00 40.06	A	0
	ATOM	519	N	ASN .		22.886	63.650	33.865	1.00 39.67	A	N
	ATOM	520	CA	ASN .		21.594	63.451	33.237	1.00 37.85	A	C
60	ATOM	521 522	CB	ASN .		20.532	64.244	35.446	1.00 37.64	A	c
00	ATOM	523		ASN .		20.013	62.606	35.695	1.00 38.24	A	ŏ
	ATOM	524		ASN .	191	20.647	64.645	36.397	1.00 35.93	A	N
	ATOM	525	C	ASN .		21.570	63.766	31.735	1.00 37.60	A	C
	ATOM	526	0	ASN .		20.518	64.003	31.150	1.00 36.22	A	0
65	ATOM	527 528	N		A 192 A 192	22.741	63.776	31.112 29.673	1.00 37.28 1.00 38.27	A	N
	ATOM ATOM	529	CB		A 192	23.511	65.351	29.873	1.00 38.46	A	c
	ATOM	530	CG2			23.623	65.488	27.795	1.00 35.81	A	C
	ATOM	531	CG1	ILE .	A 192	22.689	66.516	29.867	1.00 41.28	A	C
70	ATOM	532	CD1		A 192	23.199	67.881	29.476	1.00 38.83	A	C
	ATOM	533	C		A 192	23.672	62.881	29.108	1.00 38.70	A	C
	ATOM	534	0	ILE .	A 192	24.772	62.629	29.597	1.00 38.53	A	0

							-19-				
	ATOM	535	N	LEU	A 193	23.153	62.195	28.095	1.00 40.02	A	N
	ATOM	536	CA		A 193	23.884	61.094	27.477	1.00 39.54	A	C
	MOTA	537	CB		A 193	23.099	60.525	26.299	1.00 38.70	A	C
5	ATOM	538 539	CG CD1		A 193	23.577	59.164	25.775	1.00 38.41	A	C
,	ATOM	540	CD2		A 193 A 193	23.122	58.073 58.913	26.751 24.380	1.00 35.03	A	c
	ATOM	541	c		A 193	25.211	61.630	26.973	1.00 40.55	A	c
	MOTA	542	0		A 193	25.245	62.660	26.302	1.00 42.56	A	0
	ATOM	543	N		A 194	26.308	60.947	27.282	1.00 40.25	A	N
10	ATOM	544 545	CB		A 194 A 194	27.593 28.728	61.436 61.018	26.820 27.756	1.00 41.82 1.00 43.59	A A	C
	ATOM	545	CG		A 194	30.023	61.749	27.418	1.00 49.64	A	c
	ATOM	547	CD		A 194	31.216	61.273	28.217	1.00 56.35	A	c
	MOTA	548	NE		A 194	32.436	62.006	27.871	1.00 60.72	A	N
15	MOTA	549	CZ		A 194	33.658	61.677	28.291	1.00 64.00	A A	C
	MOTA	550 551	NH1 NH2		A 194 A 194	33.834 34.708	60.621 62.403	29.076 27.924	1.00 64.55	A	N
	MOTA	552	C		A 194	27.957	61.023	25.401	1.00 42.36	Ã	c
	MOTA	553	0	ARG	A 194	27.723	59.887	24.974	1.00 41.77	A	0
20	MOTA	554	N		A 195	28.517	61.981	24.671	1.00 41.98	A	N
	ATOM	555	CA		A 195 A 195	28.981 28.538	61.763 62.912	23.308	1.00 43.72 1.00 42.46	A	C
	ATOM	556 557	CB		A 195	28.545	62.694	20.878	1.00 46.89	A	č
	ATOM	558			A 195	28.063	63.967	20.193	1.00 48.66	A	C
25	ATOM	559			A 195	29.926	62.338	20.395	1.00 45.85	A	C
	ATOM	560	c		A 195	30.491	61.790	23.493	1.00 43.63 1.00 45.28	A A	C
	ATOM	561 562	O N		A 195 A 196	31.061 31.123	62.851 60.622	23.722 23.436	1.00 45.28 1.00 42.73	A	N
	ATOM	563	CA		A 196	32.566	60.518	23.618	1.00 44.78	A	c
30	ATOM	564	CB		A 196	32.980	59.061	23.844	1.00 46.97	A	C
	ATOM	565	CG		A 196	32.399	58.427	25.085	1.00 50.10	A	C
	ATOM	566 567	CD1 CE1		A 196 A 196	31.409 30.888	57.452 56.846	24.996 26.139	1.00 50.68 1.00 52.33	A A	c
	ATOM	568	CD2		A 196	32.853	58.786	26.352	1.00 51.97	Ä	C
35	ATOM	569	CE2	TYR	A 196	32.338	58.187	27.504	1.00 52.17	A	C
	ATOM	570	CZ		A 196	31.358	57.220	27.389	1.00 54.59	A	C
	ATOM	571 572	OH		A 196 A 196	30.844 33.356	56.626 61.070	28.525 22.443	1.00 57.15 1.00 44.49	A	0
	ATOM	573	õ		A 196	34.445	61.604	22.622	1.00 45.61	A	ŏ
40	ATOM	574	N	GLY	A 197	32.819	60.932	21.240	1.00 44.09	A	N
	ATOM	575	CA		A 197	33.517	61.441	20.074	1.00 43.41	A	С
	ATOM	576 577	0		A 197 A 197	32.913 31.804	60.907 60.380	18.797 18.802	1.00 43.77 1.00 43.31	A A	C
	ATOM	578	N		A 198	33.633	61.044	17.694	1.00 44.25	A	N
45	ATOM	579	CA	TYR	A 198	33.127	60.551	16.425	1.00 45.18	A	C
	ATOM	580	CB		A 198	32.041	61.491	15.889	1.00 49.33	A	C
	ATOM	581 582	CG CD1		A 198 A 198	32.571 33.310	62.592 63.653	14.997 15.520	1.00 55.20 1.00 57.66	A A	C
	ATOM	583	CEI		A 198	33.845	64.638	14.688	1.00 59.20	A	č
50	MOTA	584	CD2		A 198	32.375	62.543	13.618	1.00 58.31	A	C
	ATOM	585	CE2		A 198	32.904	63.521	12.775	1.00 60.71	A	C
	ATOM	586 587	OH		A 198 A 198	33.640 34.190	64.561 65.505	13.315 12.472	1.00 60.83 1.00 62.06	A	C
	ATOM	588	C		A 198	34.235	60.408	15.382	1.00 43.11	A	č
55	ATOM	589	ō		A 198	35.344	60.925	15.553	1.00 39.29	A	0
	ATOM	590	N		A 199	33.913	59.695	14.307	1.00 41.05	A	N
	ATOM ATOM	591 592	CA		A 199	34.834 35.884	59.483 58.405	13.194 13.540	1.00 42.76 1.00 41.19	A	C
	ATOM	593	CG		A 199 A 199	35.308	57.040	13.853	1.00 41.19	A	c
60	MOTA	594			A 199	35.100	56.105	12.842	1.00 42.90	A	C
	MOTA	595			A 199	35.025	56.677	15.162	1.00 40.34	A	C
	ATOM ATOM	596 597	CE1		A 199 A 199	34.623 34.545	54.822 55.394	13.129 15.465	1.00 40.61 1.00 43.97	A	C
	ATOM	598	CZ		A 199	34.345	54.464	14.441	1.00 43.37	A	c
65	MOTA	599	C	PHE	A 199	34.012	59.104	11.964	1.00 42.14	A	C
	MOTA	600	0	PHE	A 199	32.807	58.881	12.068	1.00 42.73	A	0
	MOTA	601	N		A 200		59.068	10.800	1.00 42.87	A A	N
	MOTA	602 603	CB		A 200 A 200	33.946 33.493	58.732 60.002	9.570 8.856	1.00 44.89 1.00 46.96	A	C
70	MOTA	604	CG	HIS	A 200	34.610	60.727	8.170	1.00 51.07	A	C
	ATOM	605	CD2	HIS	A 200	34.913	60.863	6.856	1.00 52.59	A	C
	MOTA	606	ND1	HIS	A 200	35.616	61.370	8.862	1.00 53.07	A	N

							-20-					
	ATOM	607	CE1 H	IIS A	200	36.489	61.870	8.005	1.00	53.71	A	C
	ATOM	608			200	36.087	61.576	6.781		52.64	A	N
	ATOM	609			200	34.838	57.969	8.597		44.12	A	C
_	ATOM	610			200	36.041	57.819	8.813 7.525		43.09 42.67	A	O N
5	ATOM	611		SP A	201	34.214	57.494 56.818	6.442		44.38	A	C
	ATOM	612 613	CA A		201 201	34.819	55.281	6.545		44.11	A	č
	ATOM	614		SP A	201	33.399	54.766	6.553		43.31	A	c
	ATOM	615		SP A	201	32.535	55.361	5.881		46.12	A	0
10	ATOM	616		SP A	201	33.152	53.742	7.222		45.46	A	0
	ATOM	617		ASP A	201	34.260	57.325	5.153		44.18	A	С
	MOTA	618		ASP A	201	33.535	58.322	5.166		42.40	A A	O
	MOTA	619			202	34.515	56.642 57.044	4.049 2.755		45.80	A	C
15	MOTA	620 621		LA A	202	33.981 34.409	56.028	1.687		44.78	A	č
13	ATOM	622		LA A		32.470	57.227	2.696		46.73	A	č
	ATOM	623			202	31.982	58.209	2.122	1.00	46.56	A	0
	ATOM	624		THR A		31.736	56.291	3.297		45.01	A	N
	ATOM	625		THR A		30.282	56.318	3.245		45.70	A	C
20	ATOM	626		PHR A	203	29.761	55.004	2.628		47.92	A	C
	ATOM	627		PHR A		29.962	53.934	3.565		50.55 46.84	A A	0
	ATOM	628		THR A		30.525 29.503	54.669 56.536	1.350		46.72	A	č
	ATOM ATOM	629 630			203	28.281	56.715	4.506		46.89	A	ŏ
25	ATOM	631		ARG A		30.170	56.528	5.699		43.86	A	N
20	ATOM	632		ARG A	204	29.424	56.680	6.948		41.61	A	С
	ATOM	633			204	29.167	55.300	7.577		42.57	A	С
	ATOM	634			204	28.645	54.199	6.646		45.37	A	c
	ATOM	635			204	28.299	52.983	7.491 6.769	1.00	52.00 59.45	A	N
30	ATOM	636 637		ARG A	204	28.122 27.200	51.719 51.489	5.838	1.00	60.63	A	Č
	MOTA	638		ARG A		26.350	52.439	5.480	1.00	63.62	A	N
	ATOM	639		ARG A	204	27.106	50.287	5.286	1.00	64.09	A	N
	ATOM	640				30.073	57.564	8.010	1.00	39.60	A	С
35	ATOM	641		ARG A		31.273	57.839	7.968	1.00	38.12	A	0
	ATOM	642		VAL A		29.249	57.993	8.967	1.00	38.69	A A	N.
	ATOM	643		VAL A	205 205	29.684 28.872	58.807 60.127	10.098 10.202	1.00	39.01	A	č
	ATOM	644 645		VAL A		29.345	60.924	11.406	1.00	37.93	A	č
40	ATOM	646		VAL A		29.031	60.957	8.919	1.00	36.49	A	C
	ATOM	647			205	29.419	57.954	11.344	1.00	36.45	A	С
	ATOM	648		VAL A		28.365	57.331	11.457	1.00	36.62	A	0
	ATOM	649		TYR A		30.367	57.911	12.271	1.00	35.58	A	C
45	ATOM	650		TYR A		30.185 31.254	57.100 55.996	13.470 13.533	1.00	40.23	A	č
45	ATOM ATOM	651 652		TYR A	206	31.301	55.101	12.314	1.00	40.95	Ã	č
	ATOM	653		TYR A		31.811	55.565	11.101	1.00	43.93	A	C
	ATOM	654		TYR A		31.859	54.741	9.973	1.00	43.38	A	Ċ
	ATOM	655		TYR A		30.836	53.784	12.372	1.00	43.86	A	C
50	ATOM	656		TYR A		30.882	52.949	11.252	1.00	42.92 43.76	A	c
	ATOM	657 658		TYR A		31.394	53.436 52.623	10.057 8.946	1.00	45.92	A	ŏ
	ATOM	659		TYR A		30.226	57.915	14.760		38.58	A	č
	ATOM	660		TYR A		31.200	58.604	15.045	1.00	40.46	A	0
55	MOTA	661		LEU A		29.163	57.823	15.544	1.00	37.67	A	N
	ATOM	662		LEU A		29.098	58.545	16.806	1.00	35.63	A	C
	ATOM	663			207	27.735	59.232	16.928	1.00	35.79 37.16	A A	C
	ATOM	664		LEU A		27.388 25.985	60.127 60.681	15.729 15.899	1.00	37.16	A	č
60	ATOM	665 666			207	28.409	61.256	15.606		33.68	Ä	č
UU	ATOM	667			207	29.314	57.561	17.955		33.49	A	C
	ATOM	668		LEU A		28.624	56.556	18.044	1.00	32.51	A	0
	ATOM	669	N	ILE A	208	30.276	57.858	18.826		31.11	A	N
	ATOM	670		ILE A		30.592	56.997	19.961	1.00	32.62	A	C
65	MOTA	671		ILE A		32.094	57.029	20.266	1.00	31.85 29.97	A	C
	ATOM	672 673		ILE A		32.423 32.889	55.991 56.759	21.298 18.983	1.00	34.87	A	c
	ATOM	674		ILE A		34.370	57.064	19.111	1.00	34.66	A	č
	ATOM	675	CDI	ILE A		29.827	57.494	21.185	1.00	33.51	A	C
70		676	0	ILE A		30.226	58.470	21.823	1.00		A	0
	ATOM	677		LEU A		28.747	56.794	21.515		32.77	A	N
	ATOM	678	CA	PEG 1	209	27.867	57.173	22.613	1.00	33.70	A	C

								-21-				
	ATOM	679	СВ	LEU	А	209	26.413	57.171	22.104	1.00 31.78	A	C
	ATOM	680	CG	LEU		209	26.089	58.037	20.880	1.00 31.51	A	C
	ATOM	681	CD1	LEU		209	24.794	57.580	20.244	1.00 32.48	A A	C
5	ATOM	682 683	CD2 C	LEU		209 209	26.011 27.933	59.504 56.314	21.295 23.878	1.00 32.96	A	č
J	ATOM	684	Ö	LEU		209	28.326	55.151	23.842	1.00 35.59	A	ō
	ATOM	685	N	GLU		210	27.529	56.917	24.993	1.00 35.23	A	N
	ATOM	686	CA	GLU		210	27.443	56.237	26.282	1.00 34.76	A	C
	MOTA	687	CB	GLU		210	27.107	57.260	27.371	1.00 36.80 1.00 37.86	A	c
10	ATOM	688 689	CC	GLU		210 210	26.610 26.086	56.678 57.752	28.686 29.637	1.00 37.86	A	c
	ATOM	690	OE1			210	25.525	57.394	30.691	1.00 38.77	A	ō
	ATOM	691	OE2			210	26.237	58.957	29.334	1.00 41.10	A	0
	ATOM	692	C			210	26.269	55.281	26.102	1.00 34.26	A	С
15	ATOM	693	0	GLU			25.304	55.624	25.417	1.00 33.07	A	0
	ATOM	694 695	N CA	TYR			26.334 25.234	54.091 53.126	26.699 26.558	1.00 34.30 1.00 32.97	A A	C M
	ATOM	696	CB	TYR			25.782	51.691	26.439	1.00 33.26	Ā	č
	ATOM	697	CG	TYR			24.709	50.628	26.361	1.00 32.75	A	С
20	ATOM	698		TYR			23.845	50.564	25.266	1.00 34.54	A	C
	ATOM	699	CE1				22.802	49.649	25.223	1.00 35.34	A A	C
	MOTA	700 701	CD2 CE2	TYR			24.507 23.461	49.732 48.807	27.414 27.385	1.00 34.61	A	č
	ATOM	702	CZ	TYR			22.609	48.774	26.288	1.00 38.58	A	č
25	ATOM	703	OH	TYR			21.538	47.896	26.267	1.00 38.81	A	0
	ATOM	704	C	TYR			24.260	53.213	27.735	1.00 33.39	A	C
	ATOM	705	0	TYR			24.671	53.179	28.894	1.00 34.96	A	N O
	ATOM	706 707	N CA	ALA			22.972 21.920	53.352 53.438	27.425 28.441	1.00 33.87	A A	C
30	ATOM	708	CB	ALA			20.919	54.559	28.080	1.00 34.05	A	č
50	ATOM	709	c	ALA	A	212	21.230	52.071	28.452	1.00 36.01	A	C
	ATOM	710	0	ALA			20.408	51.757	27.578	1.00 36.24	A	0
	ATOM	711	N	PRO			21.531	51.250	29.471 30.640	1.00 37.45 1.00 35.55	A	И
35	ATOM	712 713	CD	PRO			22.357 20.982	51.610 49.900	29.623	1.00 36.93	A	č
55	ATOM	714	CB	PRO			21.830	49.324	30.754	1.00 36.23	A	C
	ATOM	715	CG	PRO			22.033	50.511	31.627	1.00 37.14	A	С
	ATOM	716	С	PRO			19.493	49.694	29.857	1.00 37.75	A	C
40	ATOM	717	N	PRO			18.933 18.837	48.701 50.612	29.386 30.560	1.00 36.37	A A	N O
40	ATOM	718 719	CA	LEU	Ä	214	17.418	50.415	30.846	1.00 37.91	À	č
	ATOM	720	CB	LEU			17.104	50.906	32.266	1.00 36.60	A	C
	ATOM	721	CG	PEA	A	214	17.399	49.897	33.394	1.00 37.61	A	C
	ATOM	722	CD1	LEU		214	18.858	49.506	33.397	1.00 37.59	A	C
45	ATOM	723	CD2			214 214	17.028 16.371	50.497 50.939	34.736 29.859	1.00 36.22 1.00 38.39	A A	c
	ATOM	724 725	0			214	15.182	50.954	30.173	1.00 38.54	A	ŏ
	MOTA	726	N	GLY	Α	215	16.797	51.355	28.669	1.00 38.88	A	N
	MOTA	727	CA			215	15.845	51.820	27.671	1.00 39.34	A	C
50	ATOM	728	c	GLY			15.322 15.892	53.244 54.079	27.782 28.483	1.00 37.48	A	c
	MOTA	729 730	N	THR			14.226	53.517	27.079	1.00 36.14	Ã	N
	ATOM	731	CA	THR	Α	216	13.642	54.862	27.066	1.00 36.67	A	C
	MOTA	732	CB	THR			13.132	55.254	25.657	1.00 36.78	A	C
55	ATOM	733	OG1				11.980	54.461	25.327	1.00 37.06	A	0
	ATOM	734	CG2			216	14.219 12.470	55.026 55.056	24.596 28.018	1.00 34.73 1.00 36.30	A A	C
	MOTA	735 736	c			216	11.785	54.106	28.404	1.00 35.69	A	õ
	ATOM	737	N			217	12.254	56.311	28.391	1.00 38.14	A	N
60	ATOM	738	CA			217	11.147	56.686	29.258	1.00 38.24	A	C
	ATOM	739	CB			217	11.180	58.209	29.559	1.00 38.38	A A	C
	ATOM	740	CG1				9.903 12.394	58.642 58.532	30.269 30.418	1.00 38.16 1.00 34.69	A	c
	ATOM ATOM	741 742	CGZ			217	9.872	56.328	28.497	1.00 38.49	A	č
65	ATOM	743	ŏ			217	8.865	55.949	29.087	1.00 38.84	A	0
	ATOM	744	N	TYR	Α	218	9.934	56.432	27.176	1.00 39.52	A	N
	ATOM	745	CA			218	8.793	56.105	26.338	1.00 44.49 1.00 47.79	A	C
	ATOM	746 747	CB	TYR		218 218	9.128 8.037	56.352 55.903	24.868 23.932	1.00 47.79	A	c
70	ATOM	748	CDI			218	8.292	54.963	22.934	1.00 55.54	A	C
	ATOM	749	CEI	TYR	A	218	7.278	54.518	22.087	1.00 59.77	A	C
	MOTA	750	CD2	TYR	A	218	6.738	56.394	24.060	1.00 57.06	A	С

							-22-					
	ATOM	751		TYR A	218	5.714	55.957	23.219	1.00 5	9.73	A	C
	MOTA	752	CZ	TYR A		5.993	55.018	22.235	1.00 6		A	C
	MOTA	753	OH	TYR A		4.986	54.575	21.402	1.00 6		A	0
	MOTA	754	C	TYR A		8.324	54.655	26.523	1.00 4		A	C
5	ATOM	755	0	TYR A		7.131	54.409	26.740	1.00 4		A	0
	ATOM	756	N	ARG A		9.248	53.698	26.436	1.00 4		A	N
	MOTA	757	CA	ARG A		8.875	52.290	26.605	1.00 4		Α	c
	MOTA	758 759	CB	ARG A		10.059	51.355	26.324		7.75	A A	c
10	MOTA	760	CD	ARG A		9.690 10.682	49.883 48.919	26.517 25.869	1.00 5	3.31	A	c
10	ATOM	761	NE	ARG A		10.682	47.538	25.933		8.90	A	N
	ATOM	762	CZ	ARG A		10.723	46.518	25.260		0.39	A	C
	ATOM	763	NH1	ARG A		11.766	46.714	24.460		1.45	A	N
	MOTA	764	NH2	ARG A		10.199	45.301	25.382		0.62	A	N
15	MOTA	765	С	ARG A		8.349	52.033	28.015		4.03	A	C
	ATOM	766	ō	ARG A		7.381	51.297	28.202		1.33	A	o
	MOTA	767	N	GLU A	220	8.991	52.647	29.004		4.46	A	N
	MOTA	768	CA	GLU A		8.567	52.505	30.395		6.08	A	C
	ATOM	769	CB	GLU A		9.534	53.261	31.315		7.47	A	C
20	ATOM	770	CG	GLU A		9.059	53.418	32.753		2.18	A	C
	MOTA	771	CD	GLU A		10.098	54.084	33.661		5.45	A	C
	MOTA	772	OE1	GLU A		10.628	55.158	33.296		5.13	A	0
	MOTA	773	OE2			10.379	53.533	34.751		6.93	A	0
25	MOTA	774 775	C	GLU A		7.144 6.367	53.050	30.550 31.375		5.87	A	c
23	MOTA	776	N	GLU A		6.801	52.568 54.045	29.737		4.52	A A	N
	ATOM	777	CA	LEU A		5.473	54.649	29.789		5.19	A	č
	ATOM	778	CB	LEU A		5.483	55.989	29.036		5.91	A	č
	ATOM	779	CG	LEU A		4.363	57.008	29.278		7.69	A	C
30	MOTA	780	CD1	LEU A		4.268	57.346	30.755		6.44	A	C
	ATOM	781	CD2	LEU A	221	4.646	58.270	28.470	1.00 4	7.40	A	c
	ATOM	782	C	LEU A		4.465	53.674	29.170		6.08	A	C
	ATOM	783	0	LEU A		3.320	53.580	29.617		4.50	A	0
~ =	MOTA	784	N	GLN A		4.893	52.949	28.139		6.94	A	N
35	MOTA	785 786	CA	GLN A		4.715	51.960 51.299	27.505 26.313		0.56	A	C
	ATOM	787	CG	GLN A		4.715	52.143	25.069		6.98	A	c
	ATOM	788	CD	GLN A		5.281	51.318	23.882		1.40	A	č
	ATOM	789	OE1	GLN A		6.287	50.607	23.958	1.00 €		A	ō
40	MOTA	790	NE2	GLN A	222	4.542	51.403	22.776	1.00 €	1.65	A	N
	ATOM	791	C		222	3.701	50.872	28.528		0.28	A	C
	MOTA	792	0	GLN A		2.572	50.385	28.609		8.43	A	0
	MOTA	793	N	LYS A		4.718	50.502	29.301		1.04	A	N
45	MOTA	794 795	CA	LYS A		4.604 5.992	49.475 49.146	30.332 30.895	1.00 5	3.80	A	c
43	ATOM	796	CG	LYS A		6.680	47.951	30.261		7.08	A	č
	ATOM	797	CD	LYS A		6.939	48.120	28.773	1.00 5	9.58	A	č
	MOTA	798	CE	LYS A		7.506	46.821	28.187		2.45	A	С
	MOTA	799	NZ	LYS A		7.723	46.877	26.711	1.00 €	5.10	A	34
50	MOTA	800	С	LYS A		3.680	49.855	31.488		1.07	A	C
	MOTA	801	0	LYS A		2.678	49.188	31.731	1.00 5		A	0
	MOTA	802	N	LEU A		4.024	50.927	32.195		9.30	A	N
	MOTA	803	CA	LEU A		3.250	51.382	33.347		17.99	A	c
55	MOTA	804 805	CB	LEU A		4.153 5.509	52.201 51.562	34.272		15.38	A A	c
33	ATOM	806			224	6.327	52.477	35.475		3.89	A	c
	ATOM	807		LEU A		5.291	50.228	35.263	1.00 4		A	c
	ATOM	808	C	LEU A		1.979	52.183	33.067		7.57	A	č
	ATOM	809	ō	LEU A		1.198	52.417	33.986		8.98	A	ō
60	ATOM	810	N	SER A		1.770	52.596	31.818	1.00 4	17.50	Α	N
	MOTA	811	CA	SER A		0.602	53.397	31.432		6.59	A	С
	ATOM	812	CB	SER A		-0.682	52.840	32.053		18.00	A	C
	ATOM	813	OG	SER A		-1.018	51.593	31.477		1.00	A	0
65	ATOM	814 815	C	SER A		0.790 0.652	54.850 55.771	31.862 31.056		6.78	A A	0
00	ATOM	816	N	LYS A		1.113	55.043	33.136		15.76	A	N
	ATOM	817	CA	LYS A		1.349	56.371	33.690		15.69	A	C
	ATOM	818	CB	LYS A		0.019	57.049	34.025		18.92	A	ć
	ATOM	819	CG	LYS A	226	-0.896	56.251	34.937	1.00 5	0.24	A	C
70	ATOM	820	CD	LYS A		-2.286	56.871	34.944		55.99	A	00000
	ATOM	821	CE	LYS A		-3.213	56.217	35.960	1.00 5		A	
	ATOM	822	NZ	LYS A	∠26	-4.577	56.820	35.924	1.00 5	8.58	A	N

							-23-				
	ATOM	823	С	LYS A	226	2.211	56.235	34.935	1.00 43.87	A	С
	ATOM	824	0	LYS A	226	2.219	55.180	35.563	1.00 43.31	A	0
	ATOM	825	N	PHE A	227	2.945	57.291	35.280	1.00 42.51	A	N
5	ATOM	826	CB	PHE A		3.822 5.136	57.271 58.018	36.446 36.163	1.00 41.32 1.00 38.84	A A	C
3	ATOM ATOM	827 828	CG	PHE A		5.901	57.493	34.969	1.00 38.42	A	c
	ATOM	829		PHE A	227	5.793	56.155	34.574	1.00 34.24	A	c
	ATOM	830		PHE A		6.741	58.338	34.242	1.00 37.52	A	C
	ATOM	831	CE1	PHE A	227	6.506	55.673	33.477	1.00 33.25	A	c
10	ATOM	832	CE2	PHE A		7.460	57.859 56.525	33.139 32.760	1.00 37.09 1.00 31.91	A A	C
	MOTA	833 834	CZ C	PHE A		7.340 3.168	57.888	37.669	1.00 44.70	A	č
	ATOM	835	ŏ	PHE A		2.199	58.644	37.554	1.00 45.27	A	ō
	ATOM	836	N	ASP A		3.708	57.572	38.844	1.00 44.53	A	N
15	ATOM	837	CA	ASP A		3.170	58.115	40.078	1.00 45.73	A	C
	ATOM	838	CB	ASP A	228 228	3.357 4.797	57.121 57.012	41.234 41.696	1.00 47.95 1.00 50.80	A	c
	ATOM ATOM	839 840			228	5.711	57.200	40.871	1.00 55.59	A	ŏ
	ATOM	841	OD2	ASP A	228	5.016	56.718	42.889	1.00 53.57	A	0
20	ATOM	842	С	ASP A	228	3.873	59.435	40.363	1.00 44.84	A	C
	ATOM	843	0		228	4.805	59.815	39.655	1.00 42.73	A	0
	MOTA	844 845	N CA	GLU A	229 229	3.419	60.130 61.419	41.400 41.769	1.00 44.06 1.00 44.15	A	C
	ATOM	846	CB		229	3.176	62.046	42.914	1.00 46.01	Ä	č
25	ATOM	847	CG	GLU A	229	1.732	62.358	42.554	1.00 49.15	A	C
	ATOM	848	CD		229	1.149	63.475	43.398	1.00 53.31	A	C
	ATOM	849	OB1		229	1.055	63.311	44.633	1.00 54.33	A	0
	ATOM	850 851	OE2		229 229	0.785 5.459	64.525 61.412	42.823 42.146	1.00 57.15 1.00 42.45	A A	c
30	ATOM	852	ò		229	6.189	62.330	41.778	1.00 42.84	A	ő
50	ATOM	853	И	GLN A	230	5.904	60.399	42.889	1.00 42.42	A	N
	ATOM	854	CA	GLN A	230	7.309	60.355	43.291	1.00 40.75	A	С
	MOTA	855	CB	GLN A	230	7.583	59.227	44.302	1.00 43.22	A	C
35	ATOM ATOM	856 857	CD	GLN A	230	9.034	59.251 58.120	44.825 45.789	1.00 46.84 1.00 51.94	A	C
33	ATOM	858	OE1	GLN A	230	9.463	56.955	45.397	1.00 55.25	A	ŏ
	ATOM	859		GLN A		9.558	58.464	47.059	1.00 53.28	A	N
	ATOM	860	C	GLN A	230	8.233	60.171	42.095	1.00 38.22	A	С
40	ATOM	861	0	GLN A ARG A		9.274 7.851	60.816 59.286	42.014 41.176	1.00 37.20 1.00 36.78	A	N O
40	ATOM ATOM	862 863	N CA	ARG A		8.663	59.286	39.997	1.00 36.78	A	C
	ATOM	864	CB	ARG A		8.186	57.749	39.284	1.00 37.47	A	č
	ATOM	865	CG	ARG A	231	9.122	57.330	38.158	1.00 39.31	A	C
	ATOM	866	CD	ARG A		8.420	56.555	37.057	1.00 41.69	A	C
45	ATOM	867	NE	ARG A		8.185 9.134	55.146 54.213	37.380 37.466	1.00 47.47 1.00 51.32	A A	N
	ATOM	868 869	CZ NH1			8.799	52.963	37.761	1.00 52.36	Ä	N
	ATOM	870	NH2			10.416	54.515	37.266	1.00 48.44	A	N
	ATOM	871	С		231	8.635	60.192	39.013	1.00 38.58	A	C
50	ATOM	872	0	ARG A		9.640 7.477	60.497 60.836	38.381 38.878	1.00 37.91 1.00 39.25	A A	O
	ATOM ATOM	873 874	N CA	THR A		7.336	61.980	37.980	1.00 36.38	A	C
	ATOM	875	CB	THR A		5.866	62.434	37.888	1.00 35.78	A	C
	ATOM	876	OG1		232	5.077	61.377	37.327	1.00 33.52	A	0
55	MOTA	877	CG2			5.740	63.684	37.014	1.00 33.99	A	C
	MOTA	878 879	C	THR A		8.176 8.906	63.157 63.780	38.475 37.708	1.00 37.94	A	C
	ATOM	880	N	ALA A		8.085	63.445	39.769	1.00 38.61	A	N
	ATOM	881	CA	ALA A		8.820	64.556	40.364	1.00 39.65	A	C
60	ATOM	882	CB	ALA A	233	8.374	64.757	41.810	1.00 39.86	A	C
	ATOM	883	C	ALA A		10.333	64.359	40.304	1.00 39.68	A	C
	ATOM ATOM	884 885	N	ALA A		11.085 10.783	65.318 63.120	40.118	1.00 39.18 1.00 39.91	A	0
	ATOM	886	CA	THR A		12.214	62.838	40.474	1.00 39.31	A	C
65	ATOM	887	CB	THR A	234	12.517	61.360	40.828	1.00 39.65	A	C
-	ATOM	888	0G1	THR A	234	11.901	61.073	42.086	1.00 36.77	A	0
	MOTA	889	CG2			14.006	61.131	40.978	1.00 39.65	A	C
	ATOM ATOM	890 891	C	THR A		12.687 13.685	63.096 63.780	38.991 38.775	1.00 38.18	A A	0
70	ATOM	891	N	THE A		11.953	62.559	38.015	1.00 39.28	A	N
. •	ATOM	893	CA	TYR A	235	12.300	62.737	36.602	1.00 38.40	A	C
	ATOM	894	CB	TYR A	235	11.293	62.018	35.700	1.00 38.30	A	С

PCT/GB02/04589

							-24-				
	MOTA	895 896	CG	TYR .			60.517 59.853	35.606 36.209	1.00 40.28 1.00 41.54	A A	c
	ATOM	897	CEI	TYR			58.463	36.079	1.00 42.34	A	č
	ATOM	898	CD2	TYR			59.761	34.878	1.00 39.41	A	č
5	ATOM	899		TYR			58.387	34.746	1.00 40.62	A	С
	ATOM	900	CZ	TYR .			57.738	35.344	1.00 42.31	A	С
	MOTA	901	OH	TYR .			56.370	35.191	1.00 40.25	A	0
	ATOM	902	C	TYR .			64.213	36.207	1.00 38.07	A	C
10	ATOM	903	0	TYR .			64.629	35.482	1.00 36.19	A	O
10	ATOM ATOM	904 905	N CA	ILE .			65.002 66.434	36.678 36.374	1.00 39.25 1.00 37.44	A	C
	ATOM	906	CB	TLE			67.102	36.872	1.00 37.12	A	č
	ATOM	907		ILE			68,627	36.741	1.00 34.15	A	c
	ATOM	908	CG1	ILE			66.554	36.072	1.00 35.02	A	C
15	ATOM	909	CD1	ILE .			66.750	34.561	1.00 36.77	A	С
	ATOM	910	C	ILE			67.115	37.012	1.00 37.57	A	C
	ATOM	911	0	ILE			68.022	36.426	1.00 40.12	A	N
	ATOM ATOM	912 913	N CA	THR			66.668 67.215	38.209 38.891	1.00 36.62 1.00 36.77	A	C
20	ATOM	914	CB	THR		7 14.285	66.590	40.310	1.00 36.70	A	č
	ATOM	915	0G1	THR			66.970	41.134	1.00 39.88	A	ō
	ATOM	916	CG2	THR			67.072	40.970	1.00 33.73	A	С
	ATOM	917	C	THR		7 15.393	66.931	38.084	1.00 36.40	A	C
	ATOM	918	0	THR			67.808	37.917	1.00 34.72	A	0
25	ATOM	919	N	GLU			65.703	37.589	1.00 35.89	A	N
	ATOM	920 921	CB	GLU			65.343 63.831	36.826 36.584	1.00 36.31 1.00 37.43	A	c
	ATOM	922	CG	GLU			63.014	37.882	1.00 39.75	A	č
	ATOM	923	CD	GLU			61.516	37.652	1.00 42.37	A	č
30	ATOM	924	OE1				61.106	36.526	1.00 46.02	A	0
	ATOM	925	OE2	GLU	A 23	8 16.804	60.739	38.605	1.00 44.16	A	0
	ATOM	926	С	GLU	A 23	8 16.792	66.124	35.508	1.00 36.97	A	C
	ATOM	927	0	GLU	A 23	8 17.875	66.515	35.068	1.00 38.41	A	0
35	ATOM	928 929	N CA	LEU			66.371 67.133	34.898 33.646	1.00 37.50 1.00 36.81	A A	N
25	ATOM	930	CB	LEU	A 23	9 14.142	67.020	33.063	1.00 35.68	Ä	č
	ATOM	931	CG	LEU		9 13.804	65.710	32.362	1.00 39.17	A	č
	ATOM	932	CD1	LEU			65.600	32,137	1.00 37.66	A	С
	ATOM	933		LEU			65.663	31.041	1.00 37.84	A	C
40	ATOM	934	C	LEU			68.613	33.852	1.00 35.88	A	c
	ATOM	935 936	O N	LEU			69.219 69.198	33.085 34.892	1.00 34.18	A A	O
	ATOM	937	CA	ALA			70.613	35.171	1.00 37.40	A	C
	ATOM	938	CB	ALA			71.059	36.375	1.00 35.91	A	č
45	ATOM	939	C	ALA		0 17.011	70.863	35.426	1.00 37.09	A	C
	ATOM	940	0	ALA			71.896	35.024	1.00 35.00	A	0
	ATOM	941	N	ASN			69.909	36.092	1.00 38.15	A	N
	ATOM ATOM	942 943	CA	ASN ASN			70.010 68.864	36.387 37.294	1.00 37.31	A	C
50	ATOM	944	CG	ASN			69.053	38.733	1.00 39.88	A	c
50	ATOM	945	OD1				70.125	39.308	1.00 47.57	A	õ
	ATOM	946	ND2				68.006	39.331	1.00 46.92	A	N
	ATOM	947	C	ASN			69.962	35.119	1.00 36.22	A	C
	ATOM	948	0	ASN			70.724	34.975	1.00 36.76	A	0
55	ATOM	949	N	ALA			69.041	34.217	1.00 33.89	A	N C
	ATOM	950 951	CB	ALA			68.916 67.669	32.963 32.178	1.00 34.20 1.00 31.75	A	c
	ATOM	952	C	ALA			70.173	32.125	1.00 33.01	A	c
	ATOM	953	ŏ	ALA			70.719	31.574	1.00 33.65	A	ő
60	ATOM	954	N	LEU			70.630	32.043	1.00 33.50	A	N
	ATOM	955	CA	LEU	A 24	3 18.554	71.830	31.279	1.00 36.89	A	C
	ATOM	956	CB	LEU	A 24	3 17.031	71.999	31.183	1.00 34.36	A	C
	ATOM	957	CG	LEU	A 24	3 16.331 3 14.827	70.888 71.111	30.385	1.00 35.75 1.00 36.43	A A	c
65	ATOM	958 959	CD1				70.867	28.965	1.00 36.43	A	C
33	ATOM	960	CDZ	LEU			73.098	31.848	1.00 38.16	A	č
	ATOM	961	ŏ	LEU			73.956	31.083	1.00 38.31	A	ŏ
	ATOM	962	N	SER	A 24	4 19.296	73.219	33.175	1.00 39.80	A	N
	ATOM	963	CA	SER			74.391	33.778	1.00 40.44	A	C
70	ATOM	964	CB	SER			74.357	35.308	1.00 43.11	A	C
	ATOM	965 966	O.C.	SER			74.198 74.365	35.743 33.369	1.00 47.97	A A	0
	ALUM	-00	-	JAR	n 45	a 21.411	/4.305	33.309	1.00 40.05	А	-

							-25-				
	ATOM	967	0	SER A	244	22.001	75.396	33.021	1.00 40.00	A	0
	ATOM	968	N	TYR A	245	22.005	73.177	33.413	1.00 37.27	A	N
	MOTA	969	CA	TYR A		23.400	73.053	33.021	1.00 35.82	A	C
_	ATOM	970	CB	TYR A		23.897	71.622	33.252	1.00 35.21	A	C
5	ATOM	971	CG	TYR A		25.202	71.317	32.555	1.00 37.03 1.00 36.51	A A	C
	MOTA	972 973	CD1	TYR A		25.215 26.410	70.770 70.511	30.613	1.00 40.47	A	c
	ATOM	974	CD2	TYR A		26.426	71.603	33.163	1.00 38.38	A	Č
	ATOM	975	CE2	TYR A		27.630	71.350	32.507	1.00 41.25	A	Ċ
10	MOTA	976	CZ	TYR A		27.612	70.800	31.231	1.00 40.43	A	C
	MOTA	977	OH	TYR A		28.788	70.527	30.576	1.00 43.84	A	0
	MOTA	978	C	TYR A		23.561	73.448	31.550	1.00 35.32	A	C
	ATOM	979	0	TYR A		24.479	74.176	31.200	1.00 35.27	A	N O
15	MOTA	980 981	CA		246 246	22.661 22.721	72.971 73.295	30.694 29.267	1.00 36.27 1.00 38.83	A	C
13	ATOM	981	CB		246	21.609	72.568	28.498	1.00 38.59	A	č
	ATOM	983	SG	CYS A		21.897	70.797	28.263	1.00 44.30	A	s
	ATOM	984	č	CYS A	246	22.606	74.802	29.031	1.00 39.39	A	C
	MOTA	985	0	CYS A	246	23.322	75.358	28.200	1.00 37.11	A	0
20	ATOM	986	N	HIS A	247	21.704	75.461	29.756	1.00 40.65	A	N
	ATOM	987	CA	HIS A	247	21.542	76.903	29.603	1.00 43.91	A	C
	ATOM	988	CB		247	20.403	77.414	30.493	1.00 44.23 1.00 45.59	A	C
	ATOM ATOM	989 990	CCG		247 247	19.038 18.645	77.074 76.412	29.978 28.862	1.00 45.59	A	č
25	ATOM	991		HIS A		17.881	77.447	30.628	1.00 45.85	A	N
20	MOTA	992			247	16.834	77.033	29.937	1.00 46.13	A	C
	ATOM	993		HIS A		17.270	76.402	28.861	1.00 48.11	A	N
	MOTA	994	C	HIS A		22.840	77.642	29.931	1.00 46.24	A	C
	ATOM	995	0	HIS A		23.223	78.581	29.231	1.00 46.66	A	0
30	MOTA	996	N	SER A		23.527	77.213	30.985	1.00 46.80 1.00 47.62	A	C
	ATOM	997 998	CB	SER A		24.780 25.344	77.858 77.247	31.359 32.653	1.00 47.62	A	č
	ATOM	999	OG	SER A		25.872	75.950	32.432	1.00 48.53	A	ŏ
	ATOM	1000	c	SER A		25.799	77.716	30.223	1.00 47.38	A	Ċ
35	ATOM	1001	ō	SER A	248	26.774	78.469	30.152	1.00 48.22	A	0
	ATOM	1002	N	LYS A		25.566	76.761	29.328	1.00 45.39	A	N
	MOTA	1003	CA	LYS A		26.473	76.541	28.209	1.00 46.59	A	C
	ATOM	1004	CB	LYS A		26.731 27.091	75.047 74.323	28.021 29.300	1.00 44.79 1.00 49.43	A	C
40	ATOM ATOM	1005	CD	LYS A		28.337	74.902	29.951	1.00 52.06	Ã	č
-10	ATOM	1007	CE	LYS A		29.587	74.520	29.183	1.00 56.23	A	č
	MOTA	1008	NZ	LYS A		29.806	73.040	29.150	1.00 58.63	A	N
	MOTA	1009	C	LYS A		25.909	77.131	26.919	1.00 48.59	A	C
	ATOM	1010	0	LYS A		26.490	76.966	25.847	1.00 47.53	A	0
45	MOTA	1011 1012	N CA	ARG A		24.769 24.117	77.808 78.434	27.032 25.884	1.00 51.35 1.00 55.46	A A	N
	MOTA	1012	CB	ARG A		25.079	79.425	25.204	1.00 58.41	A	č
	ATOM	1014	CG	ARG A		25.543	80.543	26.151	1.00 64.68	A	č
	ATOM	1015	CD	ARG A		26.350	81.658	25.464	1.00 69.77	A	C
50	ATOM	1016	NE	ARG A		27.615	81.204	24.886	1.00 72.33	A	N
	ATOM	1017	CZ	ARG A		28.584	82.020	24.473	1.00 74.30	A A	C
	ATOM	1018	NH1	ARG A		28.439 29.699	83.338 81.520	24.574 23.951	1.00 73.90 1.00 74.27	A	N
	ATOM ATOM	1019 1020	C	ARG A		23.606	77.401	24.884	1.00 54.89	A	Č
55	ATOM	1021	ŏ	ARG A		23.589	77.635	23.671	1.00 55.10	A	ō
	ATOM	1022	N	VAL A		23.196	76.252	25.413	1.00 53.65	A	N
	ATOM	1023	CA	VAL A		22.658	75.169	24.605	1.00 51.49	A	С
	MOTA	1024	CB	VAL A		23.343	73.815	24.924	1.00 51.47	A	C
	MOTA	1025	CG1			22.550	72.664	24.310	1.00 47.16 1.00 51.44	A A	C
60	MOTA	1026 1027	CG2	VAL A		24.761 21.175	73.809 75.052	24.378 24.927	1.00 52.04	A	č
	ATOM	1027	ŏ	VAL A		20.793	74.885	26.090	1.00 50.43	A	ŏ
	ATOM	1029	N	ILE A		20.348	75.158	23.894	1.00 51.36	A	N
	ATOM	1030	CA	ILE A	252	18.908	75.050	24.049	1.00 52.79	A	C
65	MOTA	1031	CB	ILE A		18.205	76.372	23.690	1.00 54.02	A	C
	MOTA	1032	CG2			16.696	76.214	23.823	1.00 54.66	A	C
	MOTA	1033	CG1			18.709	77.490	24.611	1.00 54.46 1.00 55.53	A A	C
	MOTA	1034 1035	CD1	ILE A		18.176 18.434	78.868 73.950	24.259 23.113	1.00 53.85	A	č
70	ATOM	1036	o	ILE A		18.911	73.841	21.984	1.00 54.35	A	ŏ
. 0	ATOM	1037	N	HIS A		17.515	73.124	23.602	1.00 54.36	A	N
	MOTA	1038	CA	HIS A		16.964	72.021	22.824	1.00 54.56	A	C

								-26-					
	MOTA	1039	CB	HIS A			16.590	70.840	23.736	1.00		A	C
	MOTA	1040	CG	HIS A			17.757	70.216	24.438		52.00	A	C
	MOTA	1041		HIS A			18.281 18.546	68.970 70.907	24.359 25.334		52.22 50.80	A	C
5	ATOM	1042		HIS A			19.509	70.115	25.771		50.65	A	Č
,	ATOM	1044		HIS A			19.372	68.934	25.195		52.67	Ä	N
	ATOM	1045	C	HIS 2			15.715	72.509	22.115	1.00	55.98	A	c
	ATOM	1046	ō	HIS A	1 2	53	15.189	73.579	22.423	1.00	53.17	A	0
	ATOM	1047	N	ARG A			15.247	71.716	21.161	1.00		A	N
10	ATOM	1048	CA	ARG A			14.046	72.048	20.412	1.00		A	C
	ATOM	1049	CB	ARG A			14.391	72.384	18.956	1.00		A	C
	ATOM	1050 1051	CD	ARG A			15.314 15.366	73.592 74.081	18.803 17.357	1.00		A	č
	ATOM	1052	NE	ARG I			16.348	75.148	17.165	1.00		A	N
15	ATOM	1053	CZ	ARG 2			16.488	75.840	16.037	1.00		A	c
	ATOM	1054	NH1	ARG 2	1 2	54	15.706	75.581	14.997	1.00		A	N
	ATOM	1055		ARG 2			17.413	76.787	15.944		81.58	A	N
	ATOM	1056	С	ARG A			13.133	70.831	20.476	1.00	63.27	A	C
20	MOTA	1057	0	ARG A			13.176	69.967	19.607 21.531	1.00	65.67 60.76	A	O
20	ATOM ATOM	1058 1059	N CA		1 2		12.327 11.391	70.776 69.686	21.786		59.10	A A	C
	ATOM	1060	CB		1 2		10.512	69.404	20.549		59.56	A	č
	ATOM	1061	CG	ASP I			11.108	68.366	19.606		60.20	A	c
	MOTA	1062		ASP 2			11.300	67.208	20.026		62.58	A	0
25	MOTA	1063		ASP 2			11.372	68.702	18.433		60.34	A	0
	MOTA	1064	C	ASP 2			12.099	68.411	22.256		57.58	A	C
	MOTA	1065	0	ASP :			13.017	67.901	21.596	1.00	55.18	A A	O
	MOTA	1066 1067	N CA	ILE :			11.698 12.285	67.920 66.695	23.426 23.948	1.00		A	C
30	ATOM	1068	CB	ILE :			13.115	66.949	25.237		54.35	A	c
-	ATOM	1069		ILE :			13.581	68.397	25.271	1.00		A	Ċ
	ATOM	1070	CG1	ILE :	A 2	56	12.298	66.652	26.487	1.00		A	С
	ATOM	1071	CD1				13.151	66.501	27.717	1.00		A	Ċ
20	ATOM	1072	C	ILE :			11.150	65.705	24.193		48.66	A	C
35	ATOM ATOM	1073 1074	O	LYS I	1 2		10.242 11.190	65.957 64.598	24.989		48.97	A A	O
	ATOM	1075	CA	LYS			10.164	63.569	23.551	1.00		A	C
	ATOM	1076	CB	LYS			9.837	63.053	22.146	1.00		A	C
	ATOM	1077	CG	LYS .	A 2	57	9.671	64.158	21.119	1.00		A	C
40	ATOM	1078	CD		A 2		8.714	63.758	20.008		50.15	A	C
	ATOM	1079	CE		A 2		9.278	62.672	19.115	1.00	54.00	A	C
	ATOM	1080	NZ	LYS .	A 2		8.244 10.575	62.166 62.395	18.147 24.446		55.95 40.38	A A	N
	MOTA	1081 1082	0	LYS	1 2	57	11.761	62.170	24.688		40.25	A	ŏ
45	ATOM	1083	N	PRO			9.592	61.631	24.944		38.26	A	N
	ATOM	1084	CD	PRO .			8.141	61.822	24.769	1.00	35.77	A	C
	MOTA	1085	CA	PRO :	A 2	58	9.866	60.479	25.809		39.42	A	C
	MOTA	1086	CB	PRO .	A 2	58	8.478	59.868	26.026		38.99	A	c
50	MOTA	1087 1088	CG	PRO .	A 2	58	7.571 10.838	61.051 59.483	25.941 25.173		38.85	A A	C
50	MOTA	1088	C	PRO .			11.621	58.855	25.876	1.00	37.93	A	Ö
	MOTA	1090	N	GLU .			10.795	59.352	23.848		39.21	A	N
	ATOM	1091	CA	GLU .			11.682	58.421	23.142	1.00	39.84	A	C
	ATOM	1092	CB	GLU .			11.188	58.155	21.716	1.00	40.55	A	C
55	ATOM	1093	CG	GLU .			9.688	58.072	21.594		48.83	Α	c
	MOTA	1094	CD	GLU .			9.081	59.411	21.225		50.31	A	C
	ATOM	1095 1096		GLU .			7.919 9.776	59.679 60.190	21.604		51.19 54.44	A A	0
	ATOM ATOM	1096	C	GLU .			13.121	58.909	23.070		38.93	A	c
60	ATOM	1098	ŏ	GLU			14.011	58.149	22.694		36.58	A	ō
	ATOM	1099	N	ASN			13.347	60.176	23.413		38.55	A	N
	ATOM	1100	CA	ASN .			14.690	60.746	23.391		37.69	A	C
	ATOM	1101	CB	ASN			14.694	62.115	22.702		42.07	A	Ċ
ce	ATOM	1102	CG	ASN .			13.986 14.267	62.096	21.362		45.98 50.60	A	0
65	ATOM	1103 1104		ASN			13.062	61.258 63.032	20.507 21.171		50.14	A A	N
	ATOM	1105	C	ASN			15.222	60.883	24.818		35.15	A	C
	ATOM	1106	ŏ	ASN			16.206	61.578	25.071		33.57	A	ō
	MOTA	1107	N	LEU			14.548	60.236	25.754	1.00	32.79	A	N
70	MOTA	1108	CA	LEU	A 2	261	14.995	60.242	27.146	1.00	35.15	A	C
	ATOM	1109	CB	LEU			13.875	60.737	28.075		30.11	A	C
	ATOM	1110	CG	PEO	A 2	102	13.410	62.179	27.822	1.00	29.12	A	C

							-27-				
	MOTA	1111	CD1	LEU A	261	12.459	62.616	28.925	1.00 21.95	A	С
	MOTA	1112		LEU A		14.624	63.110	27.765	1.00 29.74	A	C
	MOTA	1113	C	TEU Y		15.366	58.785	27.462	1.00 35.15	A	C
5	MOTA	1114	O	LEU A		14.499	57.911	27.498	1.00 34.65 1.00 35.80	A	O
3	ATOM ATOM	1115 1116	CA	LEU A		16.656 17.140	58.528 57.180	27.657 27.934	1.00 35.80	A	C
	ATOM	1117	CB	LEU A		18.439	56.923	27.167	1.00 36.54	A	č
	ATOM	1118	CG	LEU A		18.311	56.713	25.654	1.00 39.58	A	C
	MOTA	1119		LEU A		19.676	56.811	25.001	1.00 37.56	A	C
10	ATOM	1120		LEU A		17.678	55.352	25.377	1.00 41.77	A	C
	ATOM	1121	C	LEU A		17.355	56.958	29.421	1.00 36.91	A	C
	ATOM	1122 1123	N	LEU A	262	17.428 17.467	57.915 55.694	30.189 29.828	1.00 38.50 1.00 36.14	A	O N
	ATOM	1123	CA	LEU A		17.640	55.364	31.246	1.00 35.96	A	Č
15	ATOM	1125	CB		263	16.472	54.488	31.709	1.00 37.11	A	C
	ATOM	1126	CG	LEU A	263	15.116	55,210	31.748	1.00 36.12	A	C
	MOTA	1127	CD1	LEU A		14.003	54.231	32.073	1.00 36.15	A	C
	ATOM	1128		LEU A		15.168	56.321	32.782	1.00 32.38	A	C
20	MOTA	1129 1130	C	LEU A		18.965 19.305	54.690 53.648	31.584	1.00 36.75 1.00 35.94	A	c
20	ATOM	1131	N	GLY A		19.700	55.301	32.512	1.00 36.23	A	N
	ATOM	1132	CA	GLY A		20.990	54.788	32.933	1.00 38.00	A	c
	ATOM	1133	C	GLY A		20.941	53.534	33.796	1.00 38.80	A	C
	MOTA	1134	0	GLY A		19.864	53.026	34.113	1.00 36.95	A	0
25	ATOM	1135	N	SER A		22.122	53.060	34.193	1.00 39.31	A	N
	ATOM	1136	CA	SER A		22.271 23.758	51.844 51.555	34.999 35.232	1.00 40.86 1.00 40.25	A	C
	ATOM	1137 1138	OG	SER A		23.750	50.288	35.847	1.00 45.33	A	Ö
	ATOM	1139	c	SER A		21.544	51.876	36.337	1.00 41.82	A	C
30	ATOM	1140	ō	SER A		21.030	50.852	36.800	1.00 43.16	A	0
	ATOM	1141	N	ALA A		21.506	53.048	36.962	1.00 43.56	A	N
	ATOM	1142	CA	ALA A		20.833	53.213	38.248	1.00 43.39	A	C
	ATOM	1143 1144	CB	ALA A		21.603 19.402	54.213 53.701	39.126 38.037	1.00 41.16	A A	c
35	MOTA MOTA	1145	0	ALA A		18.709	54.053	38.987	1.00 44.36	A	Ö
55	ATOM	1146	N	GLY A		18.960	53.722	36.787	1.00 43.26	A	N
	ATOM	1147	CA	GLY A	267	17.613	54.176	36.510	1.00 43.62	A	C
	MOTA	1148	C	GLY A		17.464	55.678	36.307	1.00 43.28	A	C
40	ATOM	1149	0	GLY A		16.346	56.156	36.114	1.00 46.43	A	O
40	MOTA MOTA	1150 1151	CA	GLU A		18.557 18.456	56.433 57.881	36.350 36.147	1.00 42.29	A	C
	ATOM	1152	CB	GLU A		19.725	58.627	36.592	1.00 44.50	Ä	č
	ATOM	1153	CG		268	20.796	57.769	37.220	1.00 50.35	A	C
	MOTA	1154	CD	GLU A	268	21.520	56.919	36.204	1.00 49.75	A	C
45	ATOM	1155		GLU A		22.583	57.358	35.701	1.00 49.51	A	0
	ATOM	1156	OE2	GLU A		21.012	55.817	35.904	1.00 48.21 1.00 41.51	A A	0
	ATOM	1157 1158	C	GLU A		18.175 18.505	58.231 57.484	34.689	1.00 41.51	A	Ö
	ATOM	1159	И	LEU A		17.563	59.390	34.502	1.00 39.23	A	И
50	ATOM	1160	CA	LEU A		17.206	59.881	33.185	1.00 38.66	A	С
	ATOM	1161	CB	LEU A		16.091	60.912	33.371	1.00 37.44	A	C
	ATOM	1162	CG	TEG Y		15.367	61.562	32.205	1.00 38.26	A	C
	ATOM	1163		LEU A		13.995 16.203	62.029 62.718	32.680 31.665	1.00 32.98 1.00 40.16	A	C
55	MOTA	1164 1165	CDZ	LEU A		18.418	60.480	32.447	1.00 36.13	Ā	č
55	ATOM	1166	ö	LEU A		19.255	61.153	33.050	1.00 34.63	A	ŏ
	MOTA	1167	N	LYS A		18.507	60.215	31.145	1.00 38.12	A	N
	MOTA	1168	CA	LYS A		19.589	60.740	30.302	1.00 38.51	A	C
	ATOM	1169	CB	LYS A		20.511	59.616	29.811	1.00 38.16	A	C
60	MOTA	1170 1171	CC	LYS A		21.125 22.288	58.721 59.391	30.874	1.00 41.06 1.00 38.38	A	C
	MOTA MOTA	1172	CE	LYS A		23.088	58.381	32.379	1.00 36.07	A	č
	ATOM	1173	NZ	LYS A		24.297	59.001	32.993	1.00 29.99	A	N
	ATOM	1174	C	LYS A	270	18.977	61.397	29.054	1.00 38.60	A	C
65	ATOM	1175	0	LYS A		18.327	60.714	28.265	1.00 38.86	A	0
	ATOM	1176	N	ILE A		19.168	62.702	28.870	1.00 36.85	A	N
	MOTA	1177 1178	CA	ILE A		18.641 18.652	63.351 64.906	27.671 27.752	1.00 38.69 1.00 38.48	A A	C
	ATOM	1179	CG2			18.141	65.498	26.426	1.00 38.13	A	C
70	ATOM	1180	CG1			17.739	65.390	28.872	1.00 37.28	A	C
	MOTA	1181	CD1	ILE A	271	17.641	66.894	28.965	1.00 41.06	A	C
	ATOM	1182	C	ILE A	271	19.579	62.934	26.547	1.00 39.33	A	C

							-28-					
	ATOM	1183	0	TLE A	271	20.761	63.273	26,562	1.00	33.34	A	0
	MOTA	1184	N	ALA A	272	19.053	62.203	25.575		43.07	A	N
	MOTA	1185	CA	ALA A		19.873	61.721	24.474		50.47	A	С
-	ATOM	1186	CB	ALA A		19.121	60.654	23.687		46.47 56.66	A	C
5	MOTA	1187	C	ALA A ALA A	272	20.320 19.630	62.829 63.837	23.539		57.25	A	0
	ATOM ATOM	1188 1189	O N	ASP A	272	21.490	62.625	22.935		61.74	A	N
	ATOM	1190	CA	ASP A	273	22.062	63.562	21.979		65.85	A	C
	ATOM	1191	CB	ASP A	273	23.107	62.837	21.120		66.61	A	С
10	ATOM	1192	CG	ASP A	273	22.680	61.413	20.754		65.34	A	C
	ATOM	1193	OD1	ASP A	273	22.571	60.579	21.679		66.75	A	0
	MOTA	1194	OD2	ASP A	273	22.457	61.118	19.561		64.24	A	0
	ATOM	1195	С	ASP A	273	20.934	64.078	21.095 20.175		69.02 69.51	A A	C
15	MOTA	1196 1197	N	ASP A PHE A	273 274	20.500	63.379 65.287	21.365		72.26	A	N
13	ATOM	1198	CA		274	19.359	65.784	20.535		74.92	A	c
	ATOM	1199	CB	PHE A	274	18.873	67.185	20.973		77.06	A	С
	ATOM	1200	CG	PHE A	274	19.908	68.278	20.889		78.54	A	С
	ATOM	1201			274	20.908	68.397	21.850	1.00	78.95	A	c
20	ATOM	1202	CD2		274	19.819	69.250	19.896 21.823	1.00	79.45 79.11	A A	c
	ATOM	1203 1204	CE1		274 274	21.797 20.700	69.480 70.330	19.861	1.00	80.03	Ä	č
	ATOM	1204	CZ	PHE A		21.691	70.448	20.828	1.00	79.54	Ã	č
	ATOM	1206	c		274	19.759	65.753	19.067	1.00	76.11	A	C
25	ATOM	1207	ō	PHE A	274	20.857	66.162	18.688	1.00	75.92	A	0
	ATOM	1208	N	GLY A	275	18.860	65.208	18.257	1.00	77.26	A	N
	ATOM	1209	CA	GLY A	275	19.106	65.096	16.836		77.96	A A	C
	ATOM	1210	C	GLY A	275	19.590 19.492	63.710 62.770	16.471 17.261		79.01	A	Ö
30	MOTA	1211 1212	N	GLY A	275 276	20.137	63.595	15.268	1.00	78.75	A	N
50	ATOM	1213	CA	TRP A	276	20.659	62.336	14.751		77.92	A	C
	ATOM	1214	CB	TRP A	276	21.944	61.930	15.489	1.00	80.84	A	С
	ATOM	1215	CG	TRP A	276	22.633	63.003	16.308	1.00	83.68	A	C
25	MOTA	1216	CD2		276	23.693	63.869	15.877	1.00	84.50 84.93	A A	C
35	ATOM ATOM	1217 1218	CE2		276 276	24.079 24.355	64.647 64.063	16.994 14.656	1.00	85.10	A	č
	MOTA	1219	CD1		276	22.420	63.289	17.627	1.00	84.53	A	č
	ATOM	1220	NE1		276	23.287	64.271	18.047	1.00	85.75	A	N
	ATOM	1221	CZ2			25.100	65.604	16.928	1.00	85.38	A	С
40	ATOM	1222	CZ3			25.373	65.018	14.592	1.00	85.86	A	C
	ATOM	1223	CH2	TRP A		25.732 19.696	65.774 61.138	15.723 14.777	1.00	85.40 75.88	A	c
	ATOM	1224 1225	C	TRP A		20.148	60.001	14.873	1.00	75.31	A	ŏ
	ATOM	1226	N	SER A		18.386	61.363	14.692	1.00	73.54	A	N
45	ATOM	1227	CA	SER A	277	17.470	60.218	14.706	1.00	69.92	A	С
	ATOM	1228	CB	SER A		16.009	60.656	14.626	1.00	69.39	A	C
	ATOM	1229	OG	SER A		15.145	59.528	14.690 13.518	1.00	68.26 68.61	A	0
	ATOM	1230 1231	C	SER A		17.795 18.330	59.324 59.791	12.514	1.00	66.97	A	Ö
50	ATOM	1232	N	VAL A		17.460	58.042	13.624	1.00	67.80	A	N
50	ATOM	1233	CA	VAL A		17.764	57.094	12.560	1.00	67.75	A	C
	MOTA	1234	CB	VAL A		18.452	55.830	13.161	1.00	67.67	A	С
	ATOM	1235	CG1			17.429	54.748	13.454	1.00	66.50	A A	c
55	ATOM	1236 1237	CG2	VAL A		19.530 16.554	55.338 56.679	11.713	1.00	68.01	A	c
33	ATOM	1237	c	VAL A		16.722	56.161	10.606	1.00	66.68	A	ŏ
	ATOM	1239	N	ALA A		15.351	56.918	12.240	1.00	69.17	A	N
	ATOM	1240	CA	ALA A	279	14.076	56.586	11.584	1.00	69.86	A	C
	ATOM	1241	CB	ALA A		14.174	56.772	10.063	1.00	69.92	A	C
60	ATOM	1242	С	ALA A		13.607	55.167	11.904	1.00	68.92 69.04	A A	C
	MOTA	1243 1244	O.	ALA A		13.970 10.838	54.593 65.378	12.929 16.485	1.00	60.42	A	N
	ATOM	1244	CA		290	9.748	65.485	17.442	1.00	58.73	À	C
	ATOM	1246	c		290	8.433	65.948	16.835	1.00	57.18	A	C
65	ATOM	1247	0	GLY A	290	8.400	66.907	16.063	1.00	56.04	A	0
	ATOM	1248	N	THR A		7.341	65.281	17.198	1.00	54.45	A	N
	MOTA	1249	CA	THR F		6.039 4.985	65.646 64.552	16.665 16.910	1.00	49.75	A	c
	MOTA	1250 1251	OGI			4.825	64.330	18.315	1.00	49.86	A	Ö
70	ATOM	1252	CG2			5.388	63.284	16.227	1.00	51.10	A	C
	ATOM	1253	c	THR A	291	5.471	66.956	17.194		46.23	A	C
	ATOM	1254	0	THR 2	291	5.959	67.548	18.163	1.00	42.68	A	0

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	MOTA	1255	N	LEU	A	292	4.419	67.386	16.514	1.00 43.51	A	N
	ATOM	1256	CA		A	292	3.696	68.601	16.819	1.00 38.04	A	C
	ATOM	1257 1258	CB		A	292 292	2.460	68.662	15.927	1.00 35.68	A	C
5	MOTA	1259	CG CD1	LEU		292	1.624 2.511	69.937 71.150	15.948 15.696	1.00 33.83 1.00 33.10	A A	c
,	ATOM	1260	CD2	LEU			0.550	69.821	14.881	1.00 35.15	A	č
	MOTA	1261	C	LEU			3.275	68.691	18.280	1.00 36.84	A	č
	ATOM	1262	0	LEU			3.286	69.771	18.862	1.00 36.40	A	0
	ATOM	1263	N	ASP		293	2.910	67.558	18.878	1.00 36.26	A	N
10		1264	CA	ASP		293	2.464	67.545	20.270	1.00 33.20	A	С
	ATOM	1265 1266	CB	ASP		293 293	2.067 0.647	66.132 65.790	20.701	1.00 36.86 1.00 37.14	A	c
	ATOM	1267	OD1				0.417	65.413	20.328 19.166	1.00 41.08	A	C
	ATOM	1268		ASP		293	-0.240	65.910	21.198	1.00 39.86	A	ŏ
15	ATOM	1269	c	ASP			3.447	68.091	21.279	1.00 32.18	A	č
	ATOM	1270	0	ASP			3.060	68.442	22.388	1.00 32.05	A	0
	ATOM	1271	N	TYR			4.719	68.170	20.920	1.00 33.09	A	N
	ATOM	1272 1273	CA	TYR			5.692 6.837	68.669 67.653	21.880 22.027	1.00 35.14 1.00 36.03	A	C
20	ATOM	1274	CG	TYR			6.352	66.274	22.443	1.00 35.56	A	č
20	MOTA	1275	CD1	TYR		294	5.804	65.389	21.509	1.00 35.20	A	č
	ATOM	1276	CE1	TYR	A	294	5.310	64.131	21.905	1.00 37.12	A	C
	ATOM	1277	CD2	TYR			6.397	65.872	23.783	1.00 35.96	A	С
0.5	ATOM	1278	CE2	TYR			5.908	64.628	24.184	1.00 34.99	A	c
25	ATOM	1279 1280	CZ OH	TYR			5.369	63.762	23.244	1.00 35.56	A	С
	ATOM	1280	C	TYR			4.917 6.245	62.521 70.064	23.644	1.00 35.68 1.00 37.52	A	0
	ATOM	1282	ŏ	TYR			7.079	70.590	22.303	1.00 39.14	A	ŏ
	ATOM	1283	N	LEU		295	5.758	70.674	20.493	1.00 36.26	A	N
30	ATOM	1284	CA	LEU	Α	295	6.232	72.005	20.102	1.00 36.64	A	C
	ATOM	1285	CB	LEU		295	6.135	72.154	18.587	1.00 35.17	A	С
	ATOM	1286 1287	CG CD1	LEU		295 295	6.953 6.675	71.141 71.328	17.781	1.00 36.95	A	c
	ATOM	1288	CD1	PEO		295	8.440	71.328	16.282 18.097	1.00 37.45	A A	c
35	ATOM	1289	c		Â	295	5.480	73.161	20.765	1.00 34.99	A	č
	ATOM	1290	ō	LEU		295	4.256	73.170	20.811	1.00 34.10	A	ō
	ATOM	1291	N	PRO		296	6.215	74.154	21.293	1.00 35.03	A	N
	MOTA	1292	CD	PRO		296	7.683	74.244	21.374	1.00 32.23	A	C
40	ATOM	1293 1294	CA	PRO		296 296	5.583 6.743	75.306 75.963	21.939	1.00 34.56	A	C
40	ATOM	1295	CG	PRO		296	7.897	75.677	22.686 21.801	1.00 32.65 1.00 35.00	A	C
	ATOM	1296	c	PRO			4.980	76.216	20.865	1.00 35.38	Ä	č
	MOTA	1297	Ó	PRO			5.423	76.210	19.715	1.00 31.51	A	ō
	ATOM	1298	N	PRO		297	3.964	77.009	21.231	1.00 35.66	A	N
45	ATOM	1299	CD	PRO			3.432	77.146	22.597	1.00 35.54	A	C
	ATOM	1300 1301	CA	PRO			3.283	77.927 78.758	20.313 21.245	1.00 36.80 1.00 37.34	A A	c
	ATOM	1302	CG	PRO			2.100	77.819	22.358	1.00 37.34	A	č
	ATOM	1303	c	PRO			4.182	78.818	19.458	1.00 37.23	A	č
50	ATOM	1304	0	PRO	A	297	3.991	78.920	18.235	1.00 33.75	A	0
	MOTA	1305	N	GLU			5.158	79.461	20.095	1.00 37.28	A	N
	ATOM	1306 1307	CA	GLU	A	298	6.040	80.368	19.375	1.00 39.04	A	c
	ATOM	1307	CB	GLU			7.016	81.072 80.146	20.335	1.00 40.64	A A	c
55	ATOM	1309	CD	GLU			7.456	79.749	22.453	1.00 41.95	A	č
	ATOM	1310	OE1	GLU			6.216	79.639	22.633	1.00 37.64	A	ō
	ATOM	1311	OE2	GLU			8.304	79.536	23.352	1.00 42.68	A	0
	ATOM	1312	C	GLU			6.805	79.668	18.266	1.00 40.93	A	С
60	ATOM	1313	0	GLU			7.175	80.297	17.272	1.00 40.31	A	0
00	ATOM	1314 1315	N CA	MET			7.029 7.759	78.366 77.624	18.415 17.395	1.00 41.73 1.00 43.83	A	N C
	ATOM	1316	CB	MET			8.495	76.437	18.017	1.00 47.01	A	č
	ATOM	1317	CG	MET			9.916	76.769	18.440	1.00 50.51	A	Č
	ATOM	1318	SD	MET	A	299	10.859	75.322	18.989	1.00 56.33	Α	s
65	MOTA	1319	CE	MET			10.979	74.398	17.460	1.00 57.30	A	C
	ATOM	1320	C	MET		299	6.907	77.157	16.222	1.00 45.51	A	C
	ATOM	1321 1322	O N	MET			7.357 5.686	77.219 76.691	15.078 16.473	1.00 46.23 1.00 46.41	A	O
	ATOM	1322	CA	ILE		300	4.857	76.691	15.354	1.00 45.41	A A	C
70	ATOM	1324	CB	ILE			3.667	75.376	15.798	1.00 48.42	A	č
	ATOM	1325	CG2	ILE	A	300	4.178	74.162	16.561	1.00 47.80	A	C
	ATOM	1326	CG1	ILE	A	300	2.709	76.179	16.675	1.00 49.64	A	С

		-30-											
	MOTA	1327		ILE A		1.559	75.360	17.234	1.00 4		A	C	
	MOTA	1328	C	ILE A		4.322	77.478	14.610	1.00 5		A A	C	
	ATOM	1329 1330	NO	ILE F		4.079	77.416 78.590	13.399 15.332	1.00 5	4.63	A	N	
5	ATOM	1331	CA	GLU 1		3.646	79.827	14.733		6.31	A	c	
,	ATOM	1332	CB	GLU I		3.129	80.780	15.815	1.00 5	64.96	A	C	
	ATOM	1333	CG	GLU F		1.744	80.422	16.350	1.00 5		A	C	
	ATOM	1334	CD		301	1.408	81.163	17.629	1.00		A	C	
10	ATOM	1335	OE1		301	2.017 0.535	82.225 80.701	17.865 18.397		57.95	A	0	
10	MOTA	1336 1337	OE2		301	4.684	80.701	13.875		6.92	A	č	
	ATOM	1338	ò		301	4.345	81.438	13.120		50.15	A	ō	
	MOTA	1339	N		302	5.943	80.119	13.988		58.80	A	N	
	ATOM	1340	CA	GLY F		6.998	80.729	13.191		9.94	A	C	
15	ATOM	1341	C	GLY I		7.683	81.921	13.838		51.59 50.55	A A	C	
	ATOM	1342 1343	N	GLY A	302	8.681 7.149	82.429 82.359	13.322 14.974		52.63	A	и	
	ATOM	1344	CA	ARG I		7.688	83.497	15.712		53.82	A	C	
	ATOM	1345	CB	ARG A		6.674	83.913	16.778	1.00	54.15	A	C	
20	MOTA	1346	CG	ARG A		5.352	84.320	16.161		55.61	A	c	
	MOTA	1347	CD	ARG A		4.180	84.153	17.100 17.925		59.14 72.61	A A	C N	
	MOTA	1348 1349	NE	ARG A		3.933 2.797	85.328 85.543	18.585	1.00	75.65	A	C	
	ATOM	1350	NH1	ARG A		2.644	86.641	19.318	1.00	75.84	Ä	N	
25	ATOM	1351	NH2	ARG A		1.806	84.660	18.509	1.00	75.29	A	N	
	ATOM	1352	C	ARG A		9.056	83.212	16.339	1.00		A	C	
	ATOM	1353	0	ARG I		9.637	82.148	16.122	1.00		A A	O	
	ATOM ATOM	1354 1355	N CA	MET I		9.572 10.871	84.173 84.038	17.099 17.756	1.00		A	C	
30	ATOM	1356	CB	MET :		11.377	85.403	18.216	1.00		A	C	
-	ATOM	1357	CG	MET :		11.911	86.312	17.135	1.00		A	C	
	MOTA	1358	SD		A 304	12.200	87.972	17.807	1.00		A	s	
	ATOM	1359	CE	MET :		13.387	87.618 83.139	19.128 18.981	1.00	78.52	A A	c	
35	ATOM ATOM	1360 1361	c	MET A	A 304	10.792 9.798	83.159	19.710		66.01	A	c	
33	ATOM	1362	N		A 305	11.847	82.361	19.216		64.22	A	N	
	ATOM	1363	CA	HIS .	A 305	11.900	81.478	20.381	1.00	63.54	A	C	
	ATOM	1364	CB		A 305	11.502	80.047	20.005		62.59	A	C	
40	ATOM	1365 1366	CG	HIS .		12.372 13.509	79.428 78.699	18.958 19.062		63.59	A	C	
40	ATOM	1366		HIS .		12.100	79.524	17.611		64.03	A	N	
	ATOM	1368		HIS .		13.031	78.878	16.930	1.00	64.73	A	C	
	MOTA	1369		HIS .		13.897	78.369	17.787		63.15	A	N	
	MOTA	1370	C		A 305	13.284	81.470	21.031		62.77	A	c	
45	MOTA	1371 1372	0		A 305 A 306	14.303 13.307	81.665 81.235	20.359		61.65 61.87	A A	N	
	ATOM ATOM	1373	N CA		A 306	14.553	81.211	23.109		59.72	A	C	
	ATOM	1374	CB		A 306	14.722	82.543	23.838	1.00	61.31	A	C	
	ATCM	1375	CG		A 306	13.804	82.668	25.035		63.77	A	C	
50	ATOM	1376		ASP .		12.597 14.293	82.368 83.073	24.903 26.111		63.61	A A	0	
	ATOM	1377 1378	C C	ASP .	A 306	14.614	80.058	24.128	1.00		A	č	
	ATOM	1379	ō		A 306	13.984	79.014	23.944	1.00	55.04	A	0	
	ATOM	1380	N	GLU	A 307	15.372	80.269	25.202	1.00	53.44	A	N	
55	ATOM	1381	CA		A 307	15.552	79.274	26.253	1.00		A	C	
	ATOM	1382 1383	CB		A 307 A 307	16.547 16.215	79.793 81.169	27.298 27.862	1.00		A	c	
	ATOM	1383	CD		A 307	15.453	81.128	29.175	1.00		A	č	
	ATOM	1385		GLU		15.048	82.215	29.646	1.00		A	0	
60	ATOM	1386	OE2		A 307	15.264	80.027	29.742	1.00		A	0	
	ATOM	1387	С		A 307	14.259	78.861	26.935 27.450	1.00		A A	c	
	MOTA	1388	O N	GLU	A 307 A 308	14.153	77.745	26.935	1.00		A	N	
	ATOM	1389 1390	CA		A 308	11.990	79.460	27.555	1.00		A	C	
65	ATOM	1391	CB	LYS	A 308	11.099	80.706	27.556	1.00		A	C	
-	ATOM	1392	CG	LYS	A 308	11.596	81.812	28.477		46.71	A	C	
	ATOM	1393	CD	LYS		11.642 12.011	81.330	29.916 30.861	1.00	46.09	A	C	
	ATOM	1394 1395	CE NZ	LYS		11.941	82.458 82.037	32.292	1.00		A	N	
70	ATOM	1395	C	LYS		11.254	78.301	26.881	1.00	39.37	A	C	
, ,	ATOM	1397	ō	LYS	A 308	10.288	77.784	27.439	1.00	38.96	A	0	
	ATOM	1398	34	VAL		11.691	77.904	25.685	1.00	37.85	A	N	

							-31-				
	ATOM	1399	CA	VAL A	309	11.055	76.781	24.999	1.00 36.62	A	С
	ATOM	1400	CB	VAL A	309	11.665	76.507	23.582	1.00 36.29	A	C
	ATOM	1401	CG1			11.361	77.654	22.638	1.00 36.56	A	c
5	ATOM ATOM	1402	CG2			13.162	76.294	23.680	1.00 36.29	A	C
,	ATOM	1403 1404	C	VAL A		11.238 10.374	75.533 74.666	25.873 25.902	1.00 36.76	A	C
	ATOM	1405	N	ASP A		12.359	75.455	26.594	1.00 37.91	A	N
	ATOM	1406	CA	ASP A		12.616	74.311	27.467	1.00 37.02	A	
	ATOM	1407	CB	ASP A		14.048	74.340	28.005	1.00 36,24	A	C
10	MOTA	1408	CG	ASP A	310	15.080	74.031	26.947	1.00 39.49	A	C
	MOTA	1409	OD1			14.820	73.177	26.074	1.00 42.74	A	0
	ATOM	1410	OD2 C	ASP A		16.172 11.633	74.629	26.994	1.00 43.52 1.00 36.95	A	0
	MOTA	1412	ŏ	ASP A		11.342	74.227 73.133	28.645 29.140	1.00 36.95 1.00 37.49	A	0
15	MOTA	1413	N		311	11.122	75.365	29.109	1.00 35.08	A	N
	MOTA	1414	CA	LEU A	311	10.166	75.333	30.211	1.00 32.22	A	C
	MOTA	1415	CB	LEU A		9.951	76.736	30.790	1.00 34.39	A	C
	MOTA	1416 1417	CG		311	10.913	77.158	31.909	1.00 33.96	A	C
20	ATOM	1418		LEU A	311	10.809 12.334	76.178 77.210	33.064 31.389	1.00 35.22 1.00 33.80	A A	C
	ATOM	1419	C	LEU A		8.833	74.752	29.743	1.00 31.56	A	č
	ATOM	1420	ō	LEU A		8.139	74.050	30.488	1.00 31.74	A	Ċ
	ATOM	1421	N	TRP A		8.466	75.048	28.503	1.00 30.35	A	N
00	ATOM	1422	CA	TRP A		7.220	74.520	27.960	1.00 29.50	A	000000
25	ATOM ATOM	1423	CB	TRP A		6.948	75.139	26.585	1.00 28.53	A	C
	ATOM	1424 1425	CG CD2	TRP A	312	5.759 4.431	74.557 75.100	25.875 25.843	1.00 28.80 1.00 30.03	A	C
	ATOM	1426	CE2		312	3.648	74.251	25.027	1.00 30.03	A	č
	ATOM	1427	CE3		312	3.830	76.225	26.421	1.00 29.90	A	č
30	ATOM	1428	CD1		312	5.730	73.429	25.103	1.00 26.36	A	С
	ATOM	1429	NE1	TRP A	312	4.460	73.237	24.589	1.00 30.47	A	N
	ATOM ATOM	1430 1431	CZ2	TRP A	312 312	2.299	74.495	24.775	1.00 32.48	A	C
	ATOM	1432	CH2		312	1.739	76.465 75.604	26.171 25.354	1.00 31.78 1.00 33.00	A	C
35	ATOM	1433	c		312	7.319	72.991	27.855	1.00 28.16	A	C C
	ATOM	1434	0		312	6.371	72.272	28.190	1.00 30.23	A	ō
	MOTA	1435	N		313	8.467	72.503	27.389	1.00 27.71	A	N
	MOTA	1436	CA	SER A	313	8.699	71.066	27.248	1.00 29.31	A	C
40	MOTA	1437 1438	CB OG	SER A		10,120 10,265	70.803 71.217	26.715 25.364	1.00 30.43	A	C
-10	ATOM	1439	C	SER A		8.540	70.373	28.605	1.00 30.79	A	c
	MOTA	1440	ō		313	7.926	69.314	28.729	1.00 31.14	A	ō
	MOTA	1441	N		314	9.101	70.994	29.628	1.00 32.96	A	N
45	MOTA	1442	CA	LEU A		9.026	70.455	30.966	1.00 33.68	A	C
45	MOTA	1443 1444	CB	LEU A	314	9.746 10.693	71.412 70.816	31.921	1.00 35.73	A	C
	ATOM	1445	CD1			11.611	69.795	32.958	1.00 39.36 1.00 37.79	A A	6
	ATOM	1446	CD2	LEU A	314	11.494	71.940	33.611	1.00 39.93	A	č
	ATOM	1447	C	LEU A		7.567	70.265	31.368	1.00 34.08	A	C
50	ATOM	1448	0	TER Y		7.213	69.270	32.002	1.00 35.54	A	0
	ATOM ATOM	1449 1450	N CA	GLY A		6.715	71,212	30.974	1.00 34.46	A	N
	ATOM	1451	C	GLY A		5.302 4.533	71.129 70.037	31.311	1.00 32.61 1.00 32.40	A	C
	ATOM	1452	ŏ	GLY A		3.653	69.393	31.156	1.00 31.59	A	Ö
55	ATOM	1453	N	VAL A		4.848	69.839	29.305	1.00 30.85	A	N
	ATOM	1454	CA	VAL A		4.191	68.812	28.500	1.00 30.81	A	C
	ATOM	1455	CB CG1	VAL A		4.675	68.870	27.019	1.00 31.13	A	C
	ATOM	1456 1457	CG1	VAL A		4.091	67.703 70.206	26.225 26.381	1.00 31.52 1.00 31.54	A	C
60	ATOM	1458	C	VAL A		4.541	67.431	29.076	1.00 30.12	A	, c
	ATOM	1459	ŏ	VAL A		3.694	66.547	29.151	1.00 28.42	A	.0
	ATOM	1460	N	LEU A	317	5.800	67.269	29.472	1.00 30.58	A	N
	ATOM	1461	CA	LEU A	317	6.307	66.018	30.041	1.00 32.76	A	C
65	ATOM	1462	CB	LEU A	317	7.834	66.091	30.182	1.00 33.36	A	C
U.S	ATOM	1463 1464		LEU A		8.741 7.959	65.504 65.186	29.091 27.838	1.00 37.19 1.00 34.20	A	000000
	ATOM	1465		LEU A		9.868	66.471	28.805	1.00 34.20	A	č
	ATOM	1466	C	LEU A	317	5.700	65.710	31.408	1.00 32.08	A	č
	ATOM	1467	0	LEU A	317	5.249	64.587	31.656	1.00.34.68	A	
70	ATOM	1468	N	CYS A	318	5.702	66.697	32.298	1.00 31.11	A	N
	ATOM	1469 1470	CA	CYS A		5.151 5.156	66.491	33.629	1.00 33.57	A	C
	WIOM	T# 10	CB	CIS A	218	3.156	67.798	34.432	1.00 33.30	A	C

							-32-				
	ATOM	1471	SG	CYS A	318	4.864	67.562	36.226	1.00 37.22	A	s
	MOTA	1472	C	CYS A		3.725	65.973	33.468	1.00 35.37	A	C
	ATOM	1473	0	CYS A		3.326	64.971	34.075	1.00 33.70 1.00 32.86	A	O
5	ATOM	1474	N CA	TYR A		2.969 1.598	66.645 66.244	32.613 32.364	1.00 32.86 1.00 33.70	A	C
,	ATOM	1476	CB	TYR A		0.927	67.239	31.395	1.00 29.85	A	č
	ATOM	1477	CG	TYR A		-0.525	66.932	31.098	1.00 30.41	A	C
	ATOM	1478	CD1			-0.877	65.857	30.276	1.00 28.02	A	C
10	ATOM	1479	CE1	TYR A		-2.207	65.545	30.022	1.00 29.18	A	C
10	ATOM	1480 1481	CD2 CE2	TYR A		-1.557 -2.902	67.696 67.387	31.667 31.424	1.00 28.95	A	c
	ATOM	1482	CZ	TYR A		-3.217	66.318	30.599	1.00 30.05	A	č
	ATOM	1483	OH	TYR A		-4.530	66.032	30.309	1.00 30.26	A	0
	ATOM	1484	C	TYR A		1.550	64.825	31.796	1.00 33.79	A	C
15	ATOM	1485	0	TYR A		0.804	63.970	32.286	1.00 34.68	A	0
	ATOM	1486	N CA		320 320	2.343	64.562 63.236	30.764 30.153	1.00 34.53 1.00 34.32	A A	N
	ATOM ATOM	1487 1488	CB		320	3.228	63.166	28.927	1.00 31.06	A	č
	ATOM	1489	CG	GLU A		3.005	61.857	28.188	1.00 40.04	A	С
20	MOTA	1490	CD	GLU A	320	3.781	61.719	26.906	1.00 42.41	A	C
	MOTA	1491	OE1	GLU A		3.546	60.713	26.203	1.00 44.86	A	0
	MOTA MOTA	1492 1493	OE2	GLU A		4.618	62.591 62.104	26.600 31.116	1.00 43.17 1.00 32.80	A A	0
	ATOM	1494	C	GLU A		2.109	61.018	31.045	1.00 32.00	A	ŏ
25	ATOM	1495	N	PHE A		3.651	62.357	32.003	1.00 32.51	A	N
	ATOM	1496	CA	PHE A		4.071	61.343	32.973	1.00 33.85	A	C
	ATOM	1497	CB	PHE A		5.235	61.833	33.829	1.00 29.43	A	c
	ATOM	1498	CG		321	6.517 6.711	62.054 61.505	33.070 31.816	1.00 30.26 1.00 28.99	A	c
30	ATOM	1499 1500	CD1		321	7.556	62.764	33.655	1.00 25.23	A	č
50	ATOM	1501	CE1		321	7.932	61.654	31.156	1.00 32.51	A	C
	ATOM	1502	CE2	PHE A	321	8.782	62.919	33.007	1.00 30.02	A	С
	ATOM	1503	cz		321	8.969	62.356	31.750	1.00 28.27	A	c
35	ATOM	1504	C	PHE A	321	2.933	60.969 59.800	33.916 34.239	1.00 36.33	A A	C
33	ATOM	1505 1506	N	LEU A		2.191	61.976	34.367	1.00 37.42	A	N
	ATOM	1507	CA	LEU A		1.085	61.755	35.296	1.00 37.42	A	c
	ATOM	1508	CB	LEU A	322	0.811	63.030	36.085	1.00 38.07	A	С
40	ATOM	1509	CG	LEU A		1.884	63.502	37.050	1.00 37.46	A	C
40	ATOM ATOM	1510 1511	CD1	LEU A		1.563	64.921 62.557	37.490 38.246	1.00 41.27 1.00 40.08	A A	C
	ATOM	1512	CDZ	LEU A		-0.214	61.302	34.658	1.00 37.12	A	č
	ATOM	1513	ŏ	LEU A		-1.004	60.596	35.281	1.00 38.55	A	0
	ATOM	1514	N	VAL A		-0.435	61.692	33.410	1.00 38.25	A	N
45	MOTA	1515	CA		323	-1.686	61.356	32.743	1.00 37.24 1.00 35.89	A	C
	ATOM ATOM	1516 1517	CB		323	-2.283 -3.556	62.634 62.300	32.058 31.285	1.00 35.08	A	č
	ATOM	1518			323	-2.587	63.683	33.123	1.00 33.83	Ä	č
	MOTA	1519	С	VAL A	323	-1.609	60.209	31.746	1.00 37.69	A	С
50	MOTA	1520	0	VAL A		-2.620	59.538	31.493	1.00 38.39	A	0
	ATOM	1521 1522	N CA	GLY A		-0.429 -0.310	59.972 58.887	31.177 30.215	1.00 36.52 1.00 38.42	A	C M
	ATOM	1523	c	GLY A		-0.333	59.333	28.759	1.00 39.62	A	č
	MOTA	1524	ō	GLY Z		-0.077	58.536	27.855	1.00 36.81	A	0
55	ATOM	1525	N	LYS A		-0.652	60.606	28.527	1.00 40.00	A	N
	ATOM	1526	CA	LYS A		-0.682	61.165	27.173	1.00 37.45	A	C
	ATOM	1527 1528	CB	LYS A		-2.002 -3.252	60.824 61.105	26.477 27.288	1.00 39.47	A A	c
	ATOM	1529	CD	LYS		-4.497	60.695	26.509	1.00 45.48	A	č
60	ATOM	1530	CE	LYS A		-5.785	61.028	27.265	1.00 49.79	A	С
	ATOM	1531	NZ	LYS A		-5.968	60.179	28.489	1.00 55.16	A	N
	ATOM	1532	C	LYS A		-0.449	62.675	27.230	1.00 33.68	A	C
	ATOM	1533 1534	O N	LYS F		-0.751 0.121	63.318 63.256	28.236 26.158	1.00 31.87 1.00 31.60	A	O
65	ATOM	1534	CD	PRO F		0.121	62.618	24.876	1.00 32.20	A	C
0.5	ATOM	1536	CA	PRO F		0.390	64.697	26.133	1.00 31.72	A	C
	ATOM	1537	CB	PRO A	326	1.174	64.879	24.832	1.00 31.00	A	C
	ATOM	1538	CG	PRO F		0.629	63.796	23.948	1.00 32.88	A	C
70	ATOM	1539 1540	C	PRO P		-0.903 -1.946	65.527 65.112	26.234	1.00 29.94	A	0
70	ATOM	1541	N	PRO 2		-0.836	66.715	26.857	1.00 27.73	A	N
	MOTA	1542	CD	PRO 7		0.377	67.360	27.400	1.00 27.90	A	c

							-33-				
	MOTA	1543	CA	PRO A 3		-2.024	67.570	27.025	1.00 29.32	A	С
	MOTA	1544	CB	PRO A 3		-1.517	68.695	27.933	1.00 25.30	A	С
	MOTA	1545	CG		327	-0.039	68.828	27.530	1.00 27.21	A	C
	ATOM	1546	C	PRO A 3	327	-2.821	68.110	25.831	1.00 30.82	A	C
5	ATOM	1547	0	PRO A 3	327	-3.998	68.441	25.988	1.00 33.12	A	0
	ATOM	1548	N	PHE A 3	328	-2.218	68.177	24.649	1.00 31.39	A	N
	ATOM	1549	CA	PHE A 3	328	-2.901	68.742	23.486	1.00 33.88	A	C
	ATOM	1550	CB	PHE A 3	328	-2.041	69.869	22.890	1.00 33.58	A	C
	ATOM	1551	CG	PHE A 3		-1.601	70.894	23.899	1.00 33.55	A	C
10	ATOM	1552		PHE A 3		-2.531	71.726	24.522	1.00 33.79	A	C
	ATOM	1553		PHE A 3		-0.257	71.002	24.256	1.00 33.06	A	C
	ATOM	1554	CE1	PHE A 3		-2.133	72.647	25.490	1.00 33.48	A	C
	ATOM	1555	CE2		328	0.160	71.923	25.226	1.00 34.56	A	C
	ATOM	1556	CZ	PHE A 3		-0.781	72.748	25.846	1.00 36.22	A	C
15	ATOM	1557	c	PHE A 3		-3.240	67.739	22.390	1.00 36.41	A	Ċ
15	ATOM	1558	ŏ		328	-3.555	68.125	21.260	1.00 36.68	A	ō
	ATOM	1559	N	GLU A 3		-3.189	66.457	22.728	1.00 39.55	A	N
	MOTA	1560	CA	GLU A 3		-3.457	65.388	21.771	1.00 42.10	A	Ĉ
	ATOM	1561	CB	GLU A 3		-3.331	64.037	22.474	1.00 44.65	A	č
20	ATOM	1562	CG		329	-3.295	62.852	21.537	1.00 51.26	A	c
20	ATOM	1563	CD	GLU A 3		-2.954	61.571	22.264	1.00 54.01	Ä	č
	ATOM			GLU A 3		-3.729	61.174	23.160	1.00 56.26	A	ő
		1564	OE2	GLU A 3		-1.907	60.966	21.943	1.00 57.24	A	ŏ
	ATOM	1565					65.498	21.089	1.00 41.21	Ä	č
00	ATOM	1566	C	GLU A 3		-4.820		21.731	1.00 38.95	A	Ö
25	ATOM	1567	0	GLU A 3		-5.827	65.795	19.783	1.00 41.49	A	N
	ATOM	1568	N	ALA A		-4.842	65.248		1.00 41.49	A	C
	MOTA	1569	CA		330	-6.077	65.330	19.014	1.00 45.23	A	č
	ATOM	1570	CB		330	-6.345	66.782	18.609		A	ć
	ATOM	1571	С		330	-6.059	64.438	17.775			0
30	MOTA	1572	0		330	-5.013	63.941	17.363	1.00 45.07	A	N
	MOTA	1573	N		331	-7.234	64.252	17.185		A	
	MOTA	1574	CA		331	-7.386	63.413	16.006	1.00 50.88	A	C
	ATOM	1575	CB		331	-8.875	63.131	15.755	1.00 54.96	A	C
	MOTA	1576	CG		331	-9.508	62.298	16.865	1.00 60.45	A	C
35	ATOM	1577	OD1		331	-9.016	61.216	17.202	1.00 64.11	A	0
	ATOM	1578	ND2	ASN A		-10.608	62.795	17.433	1.00 63.29	A	N
	ATOM	1579	C	ASN A		-6.749	63.980	14.741	1.00 49.91	A	C
	ATOM	1580	0	ASN A		-6.409	63.229	13.833	1.00 51.49	A	0
	ATOM	1581	N	THR A		-6.586	65.296	14.675	1.00 48.66	A	N
40	ATOM	1582	CA	THR A		-5.982	65.917	13.496	1.00 46.76	A	c
	ATOM	1583	CB	THR A		-7.050	66.648	12.650	1.00 47.96	A	C
	ATOM	1584	OG1	THR A		-7.648	67.696	13.424	1.00 45.93	A	0
	ATOM	1585	CG2	THR A		-8.131	65.675	12.217	1.00 46.55	A	С
	ATOM	1586	C	THR A		-4.886	66.914	13.864	1.00 44.80	A	C
45	ATOM	1587	0	THR A		-4.875	67.444	14.973	1.00 41.95	A	0
	MOTA	1588	N	TYR A		-3.954	67.155	12.940	1.00 43.86	A	N
	ATOM	1589	CA	TYR A		-2.885	68.115	13.199	1.00 43.43	A	C
	ATOM	1590	CB	TYR A		-1.938	68.232	11.999	1.00 47.91	A	C
	MOTA	1591	CG	TYR A	333	-1.084	67.015	11.710	1.00 50.72	A	C
50	MOTA	1592	CD1	TYR A	333	-1.606	65.916	11.033	1.00 53.76	A	C
	MOTA	1593	CE1	TYR A	333	-0.816	64.803	10.748	1.00 54.63	A	C
	ATOM	1594	CD2	TYR A	333	0.254	66.973	12.099	1.00 50.61	A	С
	ATOM	1595	CE2	TYR A	333	1.053	65.868	11.821	1.00 51.32	A	C
	ATOM	1596	CZ	TYR A	333	0.515	64.786	11.142	1.00 53.90	A	С
55	ATOM	1597	OH	TYR A	333	1.305	63.696	10.836	1.00 52.72	A	0
	ATOM	1598	C	TYR A	333	-3.561	69.470	13.416	1.00 42.37	A	С
	ATOM	1599	o	TYR A	333	-3.083	70.317	14.169	1.00 39.21	A	0
	ATOM	1600	N	GLN A	334	-4.688	69.643	12.734	1.00 41.68	A	N
	ATOM	1601	CA	GLN A	334	-5.479	70.865	12.790	1.00 41.47	A	C
60	ATOM	1602	CB		334	-6.709	70.733	11.885	1.00 42.29	A	С
	ATOM	1603	CG	GLN A		-7.485	72.011	11.777	1.00 45.81	A	C
	ATOM	1604	CD		334	-6.550	73.173	11.567	1.00 51.49	A	С
	MOTA	1605			334	-5.725	73.152	10.653	1.00 52.23	A	0
	MOTA	1606	NE2			-6.655	74.192	12.420	1.00 52.56	A	N
65	ATOM	1607	C	GLN A		-5.933	71.195	14.202	1.00 37.45	A	C
00	ATOM	1608	ŏ	GLN A		-5.690	72.291	14.706	1.00 33.84	A	ō
	ATOM	1609	N	GLU A		-6.599	70.231	14.821	1.00 35.59	A	N
	ATOM	1610	CA	GLU A		-7.113	70.385	16.164	1.00 37.26	A	c
	ATOM	1611	CB	GLU A	335	-8.091	69.243	16.458	1.00 39.04	A	Č
70	ATOM	1612	CG	GLU A	335	-8.854	69.370	17.767	1.00 44.38	A	č
/0	ATOM	1613	CD	GLU A	335	-9.901	70.478	17.746	1.00 49.56	A	č
	ATOM	1614	OE1			-10.579	70.666	18.784	1.00 48.54	A	ŏ
	ALON	TOT4	OET	CLU II	550	20.075	,	20.704	40.04	**	-

	-34-												
	ATOM	1615	OE2	GLU A	335	-10.042	71.159	16.699	1.00 49.52	A	0		
	ATOM	1616	C	GLU A		-5.967	70.416	17.189	1.00 36.13	A	C		
	ATOM	1617	0	GLU A		-6.083	71.062	18.232	1.00 35.59	A	0		
-	MOTA	1618	N	THR A		-4.864	69.723	16.900	1.00 33.83	A	N C		
5	ATOM	1619 1620	CB	THR A		-3.721 -2.606	69.727 68.755	17.819 17.357	1.00 32.60 1.00 31.68	A A	c		
	ATOM	1621		THE A		-3.126	67.422	17.292	1.00 34.29	A	o		
	ATOM	1622	CG2	THR A		-1.443	68,771	18.331	1.00 29.91	A	Ċ		
	ATOM	1623	c	THR A		-3.143	71.145	17.889	1.00 31.31	A	C		
10	ATOM	1624	0	THR A		-2.914	71.686	18.971	1.00 28.38	A	0		
	ATOM	1625	N	TYR A		-2.911	71.732	16.717	1.00 31.54	A	N		
	MOTA	1626	CA	TYR A		-2.381 -2.339	73.094 73.489	16.597 15.120	1.00 33.23 1.00 38.97	A	C		
	ATOM	1627 1628	CB	TYR A		-1.770	74.861	14.855	1.00 43.55	A	č		
15	ATOM	1629	CD1			-0.414	75.030	14.589	1.00 50.62	A	C		
	ATOM	1630	CE1	TYR A		0.123	76.290	14.343	1.00 53.16	A	C		
	MOTA	1631	CD2	TYR A		-2.584	75.991	14.872	1.00 43.59	A	С		
	ATOM	1632	CE2	TYR 2		-2.062	77.254	14.632	1.00 47.84	A	c		
20	ATOM	1633	CZ	TYR A		-0.704 -0.170	77.397 78.637	14.364 14.096	1.00 53.57 1.00 56.75	A	C		
20	ATOM	1634 1635	C	TYR A		-3.290	74.070	17.359	1.00 32.20	A	c		
	ATOM	1636	ŏ	TYR A		-2.823	74.890	18.159	1.00 30.91	A	ŏ		
	ATOM	1637	N		338	-4.592	73.966	17.103	1.00 30.03	A	N		
	ATOM	1638	CA	LYS F	338	-5.580	74.809	17.771	1.00 30.11	A	C		
25	ATOM	1639	CB		338	-7.008	74.344	17.421	1.00 31.44	A	С		
	ATOM	1640	CG	LYS A		-8.107	75.329 74.720	17.852 17.889	1.00 34.97 1.00 38.62	A	C		
	ATOM	1641 1642	CE	LYS A		-9.521 -10.082	74.415	16.504	1.00 43.83	A	č		
	ATOM	1643	NZ	LYS A		-11.532	74.025	16.552	1.00 43.82	A	N		
30	ATOM	1644	C	LYS A		-5.387	74.764	19.289	1.00 30.09	A	C		
	ATOM	1645	0	LYS A		-5.257	75.804	19.942	1.00 29.38	A	0		
	ATOM	1646	N	ARG A		-5.356	73.554	19.846	1.00 29.91	A	N		
	MOTA	1647 1648	CA	ARG A		-5.200 -5.376	73.370 71.880	21.288	1.00 29.88 1.00 32.35	A A	C		
35	ATOM	1649	CB		339	-6.790	71.364	21.347	1.00 37.87	A	č		
-	MOTA	1650	CD		339	-6.962	69.849	21.524	1.00 43.23	A	č		
	MOTA	1651	NE		339	-8.337	69.455	21.193	1.00 48.20	A	N		
	MOTA	1652	CZ		339	-8.845	68.223	21.287	1.00 50.25	A	C		
40	MOTA	1653 1654	NH1 NH2		339	-8.107 -10.111	67.202 68.010	21.712 20.940	1.00 48.72 1.00 51.23	A A	121 121		
40	ATOM	1655	C		339	-3.883	73.906	21.850	1.00 28.91	A	Č		
	ATOM	1656	ŏ		339	-3.853	74.491	22.930	1.00 31.71	A	ŏ		
	ATOM	1657	N	ILE 2	340	-2.792	73.700	21.125	1.00 28.62	A	N		
	ATOM	1658	CA		340	-1.487	74.180	21.565	1.00 30.14	A	C		
45	ATOM	1659	CB CG2		340	-0.366 0.932	73.660	20.631	1.00 28.04	A	C		
	ATOM	1660 1661	CG2		340	-0.190	74.397 72.142	20.807	1.00 25.38	A	c		
	ATOM	1662	CD1		340	0.830	71.531	19.845	1.00 27.76	A	C		
	ATOM	1663	C		340	-1.462	75.712	21.526	1.00 32.65	A	C		
50	ATOM	1664	0		340	-1.024	76.377	22.470	1.00 33.37	A	0		
	ATOM	1665	N	SER A		-1.935	76.243	20.404	1.00 33.83	A	C M		
	MOTA	1666 1667	CA	SER A		-2.000 -2.644	77.676 77.892	20.138 18.772	1.00 35.36	A	c		
	ATOM	1668	OG	SER A		-1.991	78.931	18.084	1.00 39.44	A	ō		
55	ATOM	1669	C	SER A	341	-2.794	78.436	21.185	1.00 35.59	A	C		
	MOTA	1670	0	SER A		-2.367	79.478	21.673	1.00 37.28	A	0		
	ATOM	1671	N		342	-3.952	77.893	21.530	1.00 34.73	A	C M		
	ATOM	1672 1673	CA	ARG A	342	-4.851 -6.296	78.508 78.295	22.493	1.00 34.53 1.00 35.36	A	c		
60	ATOM	1674	CG	ARG A		-6.539	78.913	20.641	1.00 33.30	A	č		
00	ATOM	1675	CD	ARG A		-7.836	78.460	19.969	1.00 38.01	A	č		
	ATOM	1676	NE	ARG 2		-8.038	79.214	18.730	1.00 41.54	A	N		
	ATOM	1677	CZ	ARG A		-9.135	79.184	17.974	1.00 41.67	A	C		
	ATOM	1678		ARG 2		-9.187	79.922	16.870	1.00 44.15	A	N		
65	ATOM	1679 1680	NH2 C	ARG A		-10.176 -4.652	78.435 77.962	18.315 23.900	1.00 37.28 1.00 36.18	A	C		
	ATOM	1681	0	ARG A		-5.446	78.252	24.802	1.00 34.08	A	Ö		
	ATOM	1682	N	VAL		-3.582	77.178	24.072	1.00 35.22	A	N		
	ATOM	1683	CA	VAL		-3.221	76.575	25.355	1.00 34.16	A	C		
70	MOTA	1684	CB	VAL		-2.613	77.622	26.315	1.00 34.38	A	C		
	ATOM	1685		VAL		-2.081 -1.500	76.935 78.391	27.561 25.632	1.00 36.51 1.00 31.25	A	C		
	ATOM	1686	CGZ	VAL :	1 143	-1.500	70.391	25.032	1.00 31.23	- 4	C		

							-35-				
	MOTA	1687	С	VAT.	A 343	-4.441	75.952	26.018	1.00 34.20	A	С
	ATOM	1688	o	VAL .		-4.782	76.284	27.153	1.00 31.68	A	0
	MOTA	1689	N	GLU 2		-5.097	75.050	25.294	1.00 33.81	A	N
_	MOTA	1690	CA	GLU :		-6.292	74.369	25.783	1.00 34.08	A	c
5	ATOM	1691 1692	CB	GLU .		-7.340 -8.047	74.265 75.572	24.658	1.00 34.89	A	C
	ATOM	1693	CD	GLU .		-8.665	75.594	22.944	1.00 40.26	A	č
	ATOM	1694	OE1	GLU .		-9.402	76.553	22.636	1.00 39.02	A	ŏ
	ATOM	1695	OE2	GLU .		-8.406	74.665	22.154	1.00 41.41	A	0
10	ATOM	1696	C	GLU 2		-6.022	72.972	26.337	1.00 33.90	A	C
	ATOM	1697	0	GLU .		-5.887	72.020	25.575	1.00 35.23	A	0
	ATOM	1698 1699	N CA	PHE .		-5.958 -5.736	72.851 71.558	27.661	1.00 35.80 1.00 37.65	A	N
	ATOM	1700	CB		4 345 A 345	-4.247	71.370	28.643	1.00 37.65	A	č
15	ATOM	1701	CG		A 345	-3.731	72.296	29.714	1.00 38.52	A	c
	ATOM	1702	CD1		A 345	-3.768	71.924	31.052	1.00 40.34	A	C
	ATOM	1703	CD2		A 345	-3.212	73.545	29.382	1.00 38.83	A	С
	ATOM	1704	CEI		A 345	-3.294	72.786	32.049	1.00 41.72	A A	c
20	ATOM	1705 1706	CE2		A 345 A 345	-2.737 -2.778	74.414 74.034	30.361	1.00 39.94	A	c
20	ATOM	1707	c		A 345	-6.559	71.455	29.595	1.00 39.42	A	č
	ATOM	1708	ŏ		A 345	-6.876	72.478	30.211	1.00 40.64	A	ŏ
	ATOM	1709	N	THR .	A 346	-6.905	70.225	29.985	1.00 38.79	A	N
	MOTA	1710	CA		A 346	-7.669	69.967	31.209	1.00 38.83	A	С
25	ATOM	1711	CB		A 346	-9.177	69.732	30.906	1.00 38.24	A	C
	ATOM ATOM	1712 1713	OG1 CG2	THR .	A 346 A 346	-9.324 -9.831	68.712 71.024	29.912 30.411	1.00 35.72 1.00 38.59	A	c
	ATOM	1714	C		A 346	-7.103	68.743	31.957	1.00 40.45	Ä	č
	ATOM	1715	ō	THR		-6.477	67.872	31.350	1.00 40.52	A	ŏ
30	ATOM	1716	N	PHE .	A 347	-7.337	68.684	33.267	1.00 38.41	A	N
	ATOM	1717	CA		A 347	-6.832	67.602	34.117	1.00 38.01	A	C
	ATOM	1718	CB		A 347	-6.299	68.175	35.430	1.00 33.25 1.00 37.35	A	C
	ATOM ATOM	1719 1720	CG CD1		A 347 A 347	-5.179 -3.910	69.157 68.736	35.272 34.870	1.00 37.35	A A	c
35	ATOM	1721	CD2		A 347	-5.377	70.507	35.570	1.00 35.58	Â	č
	ATOM	1722	CE1		A 347	-2.854	69.647	34.773	1.00 37.99	A	C
	MOTA	1723	CE2		A 347	-4.334	71.420	35.477	1.00 36.58	A	C
	MOTA	1724	CZ		A 347	-3.064	70.993	35.077	1.00 36.04	A	C
40	ATOM ATOM	1725 1726	C		A 347 A 347	-7.829 -8.996	66.501 66.775	34.502 34.800	1.00 40.55 1.00 40.32	A	C
40	ATOM	1727	N		A 348		65.230	34.493	1.00 40.32	A	N
	ATOM	1728	ĈD		A 348		64.654	33.855	1.00 40.80	A	С
	ATOM	1729	CA		A 348		64.177	34.887	1.00 43.29	A	С
	MOTA	1730	CB		A 348		62.888	34.612	1.00 41.59	A	С
45	ATOM	1731	CG		A 348 A 348		63.267 64.420	33.455 36.380	1.00 41.69	A A	C
	ATOM ATOM	1732 1733	C		A 348		65.136	37.003	1.00 42.10	A	ō
	ATOM	1734	N		A 349	-9.574	63.832	36.963	1.00 46.66	A	N
	ATOM	1735	CA		A 349	-9.842	64.058	38.380	1.00 49.33	A	С
50	ATOM	1736	CB		A 349	-11.171	63.396	38.774	1.00 52.46	A	С
	ATOM	1737	CG		A 349		64.001	38.043	1.00 56.47	A	C
	ATOM ATOM	1738 1739	OD1 OD2		A 349 A 349	-12.403 -13.265	65.242 63.240	37.898 37.623	1.00 56.97 1.00 59.92	A	0
	ATOM	1740	C		A 349	-8.747	63.646	39.375	1.00 49.27	A	č
55	ATOM	1741	ŏ		A 349		64.225	40.454	1.00 48.92	A	ō
	MOTA	1742	N		A 350		62.675	39.020	1.00 49.30	A	N
	MOTA	1743	CA		A 350		62.219	39.946	1.00 47.22	A	C
	MOTA	1744	CB		A 350		60.781	39.598	1.00 46.74	A	C
60	ATOM ATOM	1745 1746	CG CD1		A 350 A 350		60.649 61.141	38.287 38.135	1.00 43.91	A	C
00	ATOM	1747	CD2		A 350		60.039	37.202	1.00 40.16	A	c
	ATOM	1748	CE1		A 350		61.025	36.915	1.00 42.32	A	č
	ATOM	1749	CE2	PHE	A 350	-5.674	59.919	35.984	1.00 39.67	A	С
	ATOM	1750	$^{\rm cz}$		A 350		60.413	35.839	1.00 40.57	A	С
65	ATOM	1751 1752	C	PHE	A 350 A 350		63.085 62.876	40.109	1.00 47.01 1.00 46.65	A	C
	ATOM	1752	N	VAL			62.876	39.222	1.00 46.65	A	N
	ATOM	1754	CA	VAL			64.893	39.355	1.00 45.42	A	C
	ATOM	1755	CB	VAL			65.695	38.057	1.00 44.39	A	C
70	ATOM	1756	CG1			-2.726	66.586	38.236	1.00 40.46	A	C
	ATOM	1757	CG2				64.745	36.909	1.00 42.44	A	C
	MOTA	1758	С	VAL	A 351	-4.356	65.847	40.542	1.00 48.95	A	С

							-36-				
	ATOM	1759	0	VAL A	351	-5.391	66.498	40.709	1.00 49.11	A	0
	ATOM	1760	N	THR A		-3.304	65.913	41.355	1.00 48.97	A	N
	MOTA	1761	CA	THR A		-3.246	66.739	42.557	1.00 50.49	A	C
5	ATOM	1762 1763	CB	THR A		-2.058 -2.329	66.288 64.978	43.442	1.00 51.76 1.00 54.65	A A	C
3	MOTA	1764	0G1	THR A		-1.839	67.249	44.600	1.00 55.96	A	č
	ATOM	1765	c	THR A		-3.127	68.239	42.291	1.00 51.36	Ä	č
	ATOM	1766	ō		352	-2.633	68.655	41.240	1.00 51.12	A	0
	ATOM	1767	N	GLU A	353	-3.574	69.044	43.256	1.00 49.74	A	N
10	ATOM	1768	CA		353	-3.519	70.499	43.132	1.00 51.27	A	C
	ATOM	1769	CB		353	-4.131	71.177	44.363	1.00 53.88	A A	C
	ATOM	1770 1771	CG		353 353	-5.636 -6.446	70.993 71.598	44.533	1.00 64.09	A	č
	ATOM	1772	OE1		353	-6.082	72.700	42.921	1.00 64.63	A	ŏ
15	ATOM	1773	OE2	GLU A	353	-7.457	70.975	42.991	1.00 65.02	A	0
	MOTA	1774	C	GLU A	353	-2.088	70.989	42.969	1.00 49.88	A	C
	MOTA	1775	0		353	-1.838	71.970	42.268	1.00 50.18	A	0
	MOTA	1776	N		354	-1.154	70.319	43.635	1.00 47.30 1.00 47.27	A	C
20	MOTA	1777 1778	CA	GLY A	354 354	0.238 0.764	70.481	43.529 42.123	1.00 47.27	A	č
20	ATOM ATOM	1779	0		354	1.525	71.292	41.594	1.00 46.49	A	ŏ
	ATOM	1780	N	ALA A		0.360	69.367	41.523	1.00 45.69	A	N
	ATOM	1781	CA	ALA A	355	0.764	69.018	40.164	1.00 45.85	A	C
	ATOM	1782	CB	ALA A		0.304	67.604	39.841	1.00 43.96	A	C
25	MOTA	1783	C	ALA A		0.115	70.011.	39.194	1.00 45.34	A	C
	ATOM	1784	O N	ALA A ARG A		0.774 -1.188	70.582 70.210	38.318 39.374	1.00 43.69 1.00 44.80	A	N
	MOTA MOTA	1785 1786	CA	ARG A		-1.964	71.121	38.547	1.00 43.64	Ã	Ċ
	ATOM	1787	CB	ARG A		-3.429	71.110	39.008	1.00 43.97	A	C
30	ATOM	1788	CG	ARG A		-4.084	69.742	38.844	1.00 44.00	A	C
	MOTA	1789	CD	ARG A		-5.299	69.539	39.760	1.00 46.78	A	C
	MOTA	1790	NE	ARG A		-6.562	69.930	39.146	1.00 46.50	A	N
	MOTA	1791 1792	CZ NH1	ARG A		-7.545 -7.423	69.088 67.793	38.835 39.078	1.00 48.09 1.00 45.87	A	N
35	MOTA	1792	NH2	ARG A		-8.660	69.545	38.276	1.00 47.73	A	N
23	MOTA	1794	C	ARG A		-1.387	72.534	38.584	1.00 42.30	A	C
	ATOM	1795	ō	ARG A		-1.404	73.242	37.579	1.00 42.77	A	0
	ATOM	1796	N		357	~0.850	72.938	39.728	1.00 39.68	A	N
	MOTA	1797	CA		357	-0.273	74.267	39.836	1.00 41.20	A A	C
40	ATOM	1798	CB	ASP A	357 357	-0.047 0.628	74.645 76.002	41.305 41.454	1.00 45.03 1.00 45.48	A	c
	ATOM ATOM	1799 1800	OD1	ASP A	357	-0.080	77.030	41.454	1.00 49.20	Â	ŏ
	ATOM	1801	OD2		357	1.872	76.046	41.544	1.00 46.68	A	0
	ATOM	1802	C	ASP A	357	1.054	74.381	39.081	1.00 41.64	A	С
45	ATOM	1803	0		357	1.326	75.406	38.448	1.00 41.73	A	0
	ATOM	1804	N		358	1.888	73.343	39.153	1.00 41.39	A	N
	ATOM	1805	CA	LEU A		3.179 4.060	73.381 72.189	38.461 38.858	1.00 40.21 1.00 40.82	A	c
	MOTA MOTA	1806 1807	CB		358	5.351	71.990	38.038	1.00 39.19	Ã	č
50	MOTA	1808			358	6.262	73.211	38.156	1.00 35.41	A	Ċ
	ATOM	1809		LEU A		6.082	70.757	38.534	1.00 35.10	A	C
	MOTA	1810	C	TEO Y	358	2.989	73.376	36.949	1.00 38.71	A	C
	MOTA	1811	0	PEO Y	358	3.548	74.210	36.240	1.00 36.97	A	O
	ATOM	1812	N	ILE A	359 359	2.205 1.958	72.425 72.318	36.463 35.036	1.00 37.63 1.00 37.27	A	C
55	ATOM ATOM	1813 1814	CA	ILE A	359	1.024	71.129	34.739	1.00 35.58	A	č
	ATOM	1815	CG2			0.616	71.125	33.257	1.00 33.52	A	č
	ATOM	1816	CG1		359	1.740	69.822	35.123	1.00 33.71	A	C
	MOTA	1817	CD1			0.904	68.556	34.965	1.00 27.32	A	С
60	MOTA	1818	C	ILE A		1.367	73.619	34.490	1.00 39.28	A	C
	MOTA	1819	0	ILE A		1.756 0.448	74.080	33.419	1.00 40.17	A A	0
	MOTA	1820 1821	N CA	SER A		-0.178	74.219 75.468	35.243 34.828	1.00 39.78	A	č
	ATOM	1822	CB	SER A		-1.326	75.824	35.774	1.00 38.05	A	č
65	ATOM	1823	OG	SER A		-2.421	74.949	35.570	1.00 41.59	A	0
,,,,	ATOM	1824	C	SER A	360	0.803	76.634	34.732	1.00 38.08	A	С
	ATOM	1825	0	SER A		0.648	77.505	33.881	1.00 37.97	A	0
	MOTA	1826	N	ARG A		1.809	76.655	35.600	1.00 37.99	A	N C
70	MOTA	1827 1828	CA	ARG A		2.809 3.667	77.722 77.702	35.568 36.834	1.00 38.96 1.00 42.54	A	č
/0	ATOM	1828	CG	ARG A		2.988	78.154	38.121	1.00 50.26	A	C
	MOTA	1830	CD	ARG A		3.971	78.022	39.287	1.00 54.77	A	Ċ

							-37-				
	ATOM	1831	NE	ARG A	361	3.358	78.286	40.586	1.00 60.68	A	N
	MOTA	1832	CZ	ARG A	361	2.987	79.490	41.010	1.00 63.56	A	C
	MOTA	1833	NH1	ARG A	361	2.435	79.631	42.211	1.00 65.68	A	N
5	MOTA	1834 1835	NH2	ARG A	361 361	3.171 3.745	80.554 77.560	40.238	1.00 63.46	A A	N
,	ATOM	1836	0	ARG A	361	4.273	78.537	33.838	1.00 34.66	A	ō
	MOTA	1837	N	LEU A	362	3.956	76.314	33.966	1.00 34.75	A	N
	MOTA	1838	CA	LEU A		4.865	76.004	32.871	1.00 33.58	A	C
	MOTA	1839	CB	TEO Y	362	5.370	74.563	33.019	1.00 33.55	A	c
10	MOTA MOTA	1840 1841	CG CD1	LEU A	362 362	6.321	74.331	34.198 34.402	1.00 33.17 1.00 32.66	A	c
	ATOM	1842	CD2	LEU A		7.624	75.058	33.936	1.00 28.23	A	č
	ATOM	1843	c	LEU A		4.275	76.199	31.479	1.00 32.52	A.	č
	ATOM	1844	0	LEU A		4.965	76.657	30.580	1.00 33.69	A	0
15	MOTA	1845	N	TEO Y		3.010	75.848	31.302	1.00 29.78	A	N
	MOTA	1846	CA	LEU A	363 363	2.369	75.985 74.870	29.997 29.814	1.00 33.86 1.00 29.15	A	C
	MOTA	1847 1848	CB	TEO Y		1.323	73.401	29.868	1.00 23.15	A	č
	MOTA	1849	CD1		363	0.631	72.468	29.746	1.00 24.51	A	č
20	MOTA	1850	CD2	LEU A	363	2.837	73.123	28.748	1.00 24.89	A	С
	MOTA	1851	С	LEU A		1.726	77.371	29.798	1.00 34.25	A	C
	MOTA	1852	O N	LEU A	363	0.508 2.565	77.505 78.396	29.740 29.710	1.00 36.86 1.00 38.02	A	O N
	MOTA	1853 1854	CA	LYS A		2.117	79.773	29.510	1.00 39.26	A	C
25	ATOM	1855	CB	LYS A		2.907	80.735	30.407	1.00 40.63	A	č
	MOTA	1856	CG	LYS A	364	2.650	80.605	31.901	1.00 42.73	A	С
	MOTA	1857	CD	LYS A		1.227	81.004	32.237	1.00 45.77	A	C
	ATOM	1858 1859	CE	LYS A	364	1.046	81.228 81.742	33.725 34.024	1.00 50.52 1.00 54.71	A	C
30	ATOM	1860	C	LYS A		2.372	80.145	28.057	1.00 39.30	A	C
50	ATOM	1861	ŏ	LYS A		3.496	79.997	27.569	1.00 38.57	A	0
	ATOM	1862	N	HIS A	365	1.335	80.616	27.368	1.00 39.57	A	N
	ATOM	1863	CA	HIS A		1.476	81.020	25.970	1.00 40.20	A	c
35	ATOM	1864 1865	CB	HIS A	365 365	0.187	81.659 82.111	25.451 24.027	1.00 40.44 1.00 37.64	A	C
33	ATOM	1866		HIS A		0.827	83.219	23.477	1.00 40.32	λ	č
	ATOM	1867			365	-0.179	81.349	22.974	1.00 38.59	A	N
	MOTA	1868		HIS A		0.088	81.963	21.836	1.00 36.60	A	С
40	MOTA	1869			365	0.699	83.101	22.113 25.839	1.00 41.15 1.00 40.73	A A	N
40	MOTA	1870 1871	C		365	2.606	82.031 81.948	24.925	1.00 40.73	A	Ö
	MOTA	1872	N		366	2.637	82.997	26.753	1.00 42.45	A	N
	MOTA	1873	CA		366	3.681	84.024	26.737	1.00 44.24	A	С
	MOTA	1874	CB		366	3.183	85.272	27.477	1.00 44.55	A	C
45	MOTA	1875	CG	ASN A		4.149	86.454 87.591	27.384 27.682	1.00 47.76 1.00 51.08	A	C
	ATOM	1876 1877	OD1 ND2		366	5.388	86.194	26.985	1.00 43.49	A	N
	MOTA	1878	C	ASN A		4.922	83.443	27.415	1.00 42.19	A	C
	MOTA	1879	0	ASN A		4.885	83.105	28.594	1.00 39.81	A	0
50	ATOM	1880	N	PRO A		6.036	83.321	26.668	1.00 44.23 1.00 43.04	A	N
	ATOM	1881 1882	CD	PRO A		6.151 7.319	83.761 82.778	25.267 27.145	1.00 43.04 1.00 45.24	A	c
	ATOM	1883	CB	PRO A		8.252	82.989	25.953	1.00 44.30	A	č
	ATOM	1884	CG	PRO A		7.320	82.944	24.778	1.00 45.18	A	С
55	ATOM	1885	С	PRO A		7.851	83.444	28.413	1.00 47.56	A	C
	MOTA	1886	0	PRO A		8.370	82.764	29.312	1.00 46.80 1.00 47.18	A	O N
	MOTA	1887 1888	N CA	SER A		7.716 8.162	84.770 85.579	28.470 29.607	1.00 47.18	A	C
	ATOM	1889	СВ	SER A		7.926	87.076	29.334	1.00 48.23	A	č
60	ATOM	1890	OG	SER A	368	8.681	87.537	28.227	1.00 51.49	A	0
	MOTA	1891	C		368	7.447	85.211	30.897	1.00 46.18	Α	С
	MOTA	1892 1893	N O		368	7.988 6.228	85.406 84.699	31.989 30.787	1.00 48.13 1.00 45.87	A A	O
	MOTA	1893	CA	GLN A		5.481	84.329	31.984	1.00 47.80	A	C
65	ATOM	1895	CB		369	3.973	84.295	31.697	1.00 51.34	A	C
	MOTA	1896	CG	GLN A	369	3.343	85.642	31.358	1.00 53.45	A	С
	MOTA	1897	CD		369	1.840	85.530	31.120	1.00 57.46	A	c
	MOTA	1898 1899	OE1 NE2	GLN A	369	1.061	85.287 85.698	32.048 29.872	1.00 60.02 1.00 58.61	A	O N
70	ATOM	1900	C	GLN A		5.916	82.983	32.561	1.00 47.67	λ	C.
	ATOM	1901	ŏ	GLN A		5.606	82.668	33.715	1.00 46.25	A	0
	MOTA	1902	N	ARG A	370	6.628	82.188	31.765	1.00 46.58	A	N

							-38-					
	MOTA	1903	CA	ARG I		7.095	80.881	32.229		47.27	A	С
	ATOM	1904	CB	ARG I		7.596	80.040	31.042		43.84	A	c
	MOTA	1905	CG	ARG I		6.520	79.778	29.989 28.732		41.08	A A	c
5	MOTA	1906 1907	CD NE	ARG I	A 370	7.094 6.191	79.136 79.264	27.585		38.83	A	N
,	ATOM	1908	CZ		A 370	6.563	79.083	26.324	1.00	36.60	A	c
	ATOM	1909		ARG I		7.816	78.757	26.039	1.00	35.02	A	N
	ATOM	1910	NH2	ARG 2		5.692	79.264	25.343		37.82	A	N
	ATOM	1911	C	ARG A		8.209	81.119	33.247		47.29	A	C
10	ATOM	1912 1913	0	PRO		8.995 8.284	82.057 80.277	33.102 34.296		48.42	A	O N
	MOTA	1914	CD	PRO I		7.383	79.135	34.552		46.07	A	C
	ATOM	1915	CA	PRO		9.291	80.382	35.359		46.72	A	c
	ATOM	1916	CB	PRO 2		8.772	79.410	36.415		45.48	A.	C
15	MOTA	1917	CG	PRO 2		8.160	78.338	35.581		47.78	A	C
	ATOM	1918	C		A 371	10.734	80.076	34.980		47.35	A	c
	MOTA	1919 1920	N.	PRO MET	A 371 A 372	11.026 11.642	79.618 80.357	33.877 35.911		47.37	A A	N
	MOTA	1921	CA		A 372	13.055	80.067	35.713		47.91	Ā	c
20	ATOM	1922	CB		A 372	13.923	80.961	36.598		51.73	A	С
	ATOM	1923	CG		A 372	13.788	82.444	36.324		56.54	A	C
	MOTA	1924	SD		A 372	14.948	83.405	37.339	1.00	60.67	A	S
	MOTA	1925	CE		A 372	16.321	83.556	36.190		59.45 45.14	A	C
25	MOTA	1926 1927	C		A 372 A 372	13.178 12.344	78.618 78.139	36.164 36.929		44.11	A	Ö
دع	MOTA	1928	M O		A 373	14.204	77.917	35.703		44.75	A	N
	ATOM	1929	CA		A 373	14.354	76.522	36.086	1.00	44.46	A	C
	ATOM	1930	CB	LEU .	A 373	15.526	75.893	35.325	1.00	42.40	A	C
	ATOM	1931	CG		A 373	15.209	75.530	33.861		41.97	A	c
30	MOTA	1932	CD1		A 373 A 373	16.493 14.223	75.194 74.352	33.117 33.808		37.82	A	C C
	MOTA MOTA	1933 1934	CD2 C		A 373 A 373	14.223	76.353	37.597	1.00	44.43	A	č
	MOTA	1935	ŏ		A 373	14.051	75.364	38.164	1.00	43.69	A	ŏ
	MOTA	1936	N		A 374	15.121	77.336	38.249	1.00	47.31	A	N
35	MOTA	1937	CA		A 374	15.310	77.289	39.699	1.00	48.80	A	C
	MOTA	1938	CB		A 374	16.126	78.496	40.152	1.00	49.01	A A	c
	ATOM ATOM	1939 1940	C	ALA ALA	A 374 A 374	13.967 13.825	77.239 76.527	40.446	1.00	49.34	A	c c
	ATOM	1941	N		A 375	12.981	77.986	39.960	1.00	50.02	A	N
40	ATOM	1942	CA		A 375	11.662	78.006	40.582	1.00	50.79	A	C
	ATOM	1943	CB		A 375	10.785	79.070	39.925	1.00	53.29	A	С
	ATOM	1944	CG		A 375	11.341	80.477	39.993	1.00	58.36	A	c
	ATOM	1945	CD		A 375 A 375	10.491 9.294	81.460 81.606	39.207 39.540	1.00	60.16	A A	Ö
45	ATOM	1946 1947	OE1		A 375	11.015	82.078	38.255	1.00	59.36	A	ŏ
75	ATOM	1948	C		A 375	10.954	76.653	40.485	1.00	50.97	A	Ċ
	ATOM	1949	0	GLU	A 375	10.032	76.373	41.253	1.00	50.08	A	0
	MOTA	1950	N		A 376	11.363	75.826	39.526	1.00	50.81	A	N
	MOTA	1951	CB		A 376 A 376	10.765	74.502 73.942	39.358 37.927	1.00	50.86 51.95	A A	c
50	MOTA	1952 1953	CG1		A 376	10.995 10.460	72.511	37.836	1.00	49.77	A	č
	ATOM	1954	CG2		A 376	10.306	74.834	36.895	1.00	50.95	A	Ċ
	MOTA	1955	C	VAL	A 376	11.379	73.524	40.360	1.00	50.64	A	C
	MOTA	1956	0		A 376	10.682	72.682	40.928	1.00	51.15	A	0
55	ATOM	1957	N	LEU	A 377	12.687	73.642	40.564	1.00	50.28	A	N C
	MOTA	1958 1959	CB	LEU	A 377 A 377	13.413 14.921	72.782 72.951	41.492 41.294	1.00	52.39	A	c
	ATOM	1960	CG		A 377	15.497	72.434	39.973	1.00	49.77	A	č
	ATOM	1961			A 377	16.942	72.875	39.830	1.00	47.65	A	C
60	ATOM	1962	CD2		A 377	15.393	70.919	39.931	1.00	48.67	A	С
	ATOM	1963	C		A 377	13.054	73.091	42.944	1.00	54.42	A	c
	MOTA	1964	0	LEU		13.302	72.283	43.841	1.00	55.25 55.92	A	N
	MOTA MOTA	1965 1966	N CA		A 378 A 378	12.467 12.075	74.263 74.676	43.169 44.510	1.00	56.51	A	C
65	ATOM	1967	CB	GLU		12.597	76.079	44.791	1.00	57.88	A	C
0.0	MOTA	1968	CG	GLU	A 378	14.102	76.137	44.929	1.00	61.78	A	C
	MOTA	1969	CD	GLU		14.631	77.545	44.819	1.00	65.68	A	C
	MOTA	1970	OE1			15.846	77.741	45.039	1.00	68.31 67.56	A A	0.
70	MOTA	1971 1972	OE2	GLU		13.834	78.456 74.639	44.502 44.721	1.00	55.69	A	č
70	ATOM	1972	Ö	GLU		10.081	75.016	45.784	1.00	57.50	A	ŏ
	ATOM	1974	N		A 379	9.832	74.183	43.715		52.52	A	N -

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	ATOM	1975	CA	HIS	A	379	8.381	74.103	43.824	1.00	50.30	A	С
	ATOM	1976	CB			379	7.773	73.684	42.484		46.98	A	C
	ATOM	1977	CG			379	6.276	73.759	42.441		45.89	A	C
_	ATOM	1978				379	5.446	74.721	41.969		43.25	A	C
5	ATOM	1979		HIS			5.463 4.197	72.753 73.090	42.922 42.746		44.60	A	N
	ATOM	1980 1981		HIS			4.159	74.279	42.170		45.42	A	N
	ATOM	1982	C	HIS			8.002	73.108	44.918		51.08	A	Ĉ
	ATOM	1983	ō	HIS			8.526	71.992	44.975	1.00	50.77	A	0
10	ATOM	1984	N	PRO	A	380	7.076	73.506	45.804		52.09	A	N
	MOTA	1985	CD	PRO			6.283	74.747	45.721		52.19	A	C
	MOTA	1986	CA	PRO			6.612	72.669	46.913	1.00	50.97	A	C
	ATOM	1987	CB	PRO			5.502 5.003	73.519 74.343	47.546 46.401	1.00	51.57 53.46	A A	c
15	ATOM	1988 1989	CG	PRO			6.146	71.257	46.549		49.66	A	č
13	ATOM	1990	ŏ	PRO			6.253	70.340	47.361		48.94	A	ō
	ATOM	1991	N	TRP			5.626	71.074	45.341	1.00	47.98	A	N
	ATOM	1992	CA			381	5.169	69.751	44.936		46.47	A	С
	ATOM	1993	CB			381	4.188	69.854	43.774		45.54	A	C
20	ATOM	1994	CG			381	3.631	68.527	43.346		40.93	A	C
	ATOM ATOM	1995 1996	CD2 CE2			381 381	4.049	67.743 66.595	42.222 42.185		38.42	A	č
	ATOM	1997	CE3				5.036	67.900	41.238		40.44	A	č
	ATOM	1998		TRP			2.606	67.840	43.932		41.28	A	С
25	MOTA	1999	NE1				2.356	66.681	43.240		40.02	A	N
	MOTA	2000	CZ2				3.359	65.605	41.200		38.16	A	c
	ATOM	2001		TRP			5.167	66.914 65.783	40.257		39.27	A	C
	MOTA	2002	CH2	TRP			4.332 6.362	68.898	44.516		46.87	A	č
30	ATOM	2003	o	TRP			6.373	67.683	44.718		46.53	A	ō
50	ATOM	2005	N	ILE			7.362	69.539	43.917	1.00	48.95	A	N
	ATOM	2006	CA		A	382	8.566	68.835	43.485	1.00	50.95	A	C
	ATOM	2007	CB	ILE			9.489	69.749	42.634		49.30	A	0 0 0
35	ATOM	2008	CG2				10.821	69.053 70.098	42.398 41.294		48.74	A A	c
33	ATOM ATOM	2009 2010	CG1				8.822 8.619	68.907	40.358		42.81	A	C
	ATOM	2011	CDI	ILE		382	9.341	68.384	44.725		53.01	A	č
	ATOM	2012	ŏ	ILE		382	9.651	67.203	44.889		51.75	A	0
	ATOM	2013	N	THR			9.643	69.340	45.596		56.54	A	N
40	ATOM	2014	CA	THR			10.384	69.069	46.827		60.42	A	C
	MOTA	2015	CB	THR			10.615 11.390	70.364 71.279	47.629 46.844		60.63	A	0
	ATOM	2017	CG2				11.360	70.067	48.923		64.67	Ã	č
	ATOM	2018	C	THR			9.667	68.070	47.726	1.00		A	C
45	ATOM	2019	ō	THR			10.303	67.355	48.501	1.00	62.87	A	0
	ATOM	2020	N	ALA			8.346	68.010	47.609	1.00	61.81	A	N
	ATOM	2021	CA	ALA			7.554	67.104	48.427 48.585	1.00		A A	C
	ATOM ATOM	2022	CB	ALA ALA			6.140 7.493	67.656 65.668	47.909	1.00		A	č
50	ATOM	2024	ŏ	ALA	Α	384	7.337	64.735	48.695	1.00		Ã	ŏ
	ATOM	2025	N	ASN	A	385	7.612	65.482	46.597	1.00	62.18	A	N
	ATOM	2026	CA	ASN			7.550	64.140	46.025	1.00	62.42	A	C
	MOTA	2027	CB	ASN			6.466	64.083	44.946	1.00	61.14	A	C
55	ATOM	2028 2029	CG	ASN			5.078 4.427	64.372 63.499	45.491 46.065		57.45	A	ő
33	ATOM	2029		ASN			4.623	65,610	45.317		56.76	Ã	N
	ATOM	2031	c	ASN			8.871	63.653	45.430	1.00	63.75	A	C
	ATOM	2032	0	ASN			9.030	62.466	45.154	1.00	63.17	A	0
	ATOM	2033	N	SER			9.814	64.565	45.234		66.08	A	N
60	ATOM	2034	CA	SER			11.103	64.211	44.651 43.990		69.04 70.22	A	C
	ATOM	2035 2036	CB	SER			11.731 13.032	65.441 65.159	43.503		70.59	A	ō
	ATOM	2036	c	SER			12.093	63.626	45.654		72.01	A	č
	ATOM	2038	ŏ	SER	A	386	12.098	63.989	46.833		73.11	A	0
65	ATOM	2039	N	SER	Α	387	12.931	62.717	45.169	1.00	73.40	A	N
	MOTA	2040	CA	SER			13.951	62.088	45.995	1.00	75.94	A	c
	ATOM	2041	CB	SER		387 387	14.024 12.754	60.589 59.981	45.695 45.840	1.00	75.91 76.94	A A	C
	ATOM ATOM	2042 2043	OG	SER		387	15.284	62.751	45.650	1.00	77.73	A	č
70	ATOM	2043	ö	SER			16.348	62.280	46.058	1.00		A	0
. •	ATOM	2045	N	LYS	Α	388	15.194	63.843	44.886		78.26	A	N
	ATOM	2046	CA	LYS	A	388	16.339	64.635	44.428	1.00	79.08	A	C

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	ATOM	2047	CB LYS A 388	17.409	-40- 64.724	45.525	1.00 79.44	A	С
	ATOM	2048	CG LYS A 388	16.974	65.500	46.763	1.00 79.33	A	č
	ATOM	2049	CD LYS A 388	18.062	65.484	47.824	1.00 79.09	A	č
	ATOM	2050	CE LYS A 388	17.695	66.350	49.018	1.00 79.02	A	C
5	ATOM	2051	NZ LYS A 388	17.530	67.782	48.641	1.00 78.19	A	N
	ATOM	2052	C LYS A 388	16.959	64.102	43.130	1.00 78.82	A	c
	MOTA	2053	O LYS A 388	16.481 17.916	63.074	42.619	1.00 78.44	A	0
	ATOM ATOM	2054	OXT LYS A 388 PB AANP Z 379	15.037	64.723 57.738	42.618 17.969	1.00 79.61 0.50 47.69	A Z	P
10	MOTA	2050	PR BANP Z 379	17.785	58.350	20.389	0.50 50.58	z	P
10	MOTA	2058	Olbaanp z 379	15.506	57.453	19.308	0.50 49.57	ž	õ
	MOTA	2059	O1BBANP Z 379	18.803	57,539	21.023	0.50 51.23	z	ō
	ATOM	2060	O2BAANP Z 379	14.617	59.160	17.829	0.50 48.87	Z	0
	ATOM	2061	O2BBANP Z 379	18.020	59.811	20.601	0.50 52.85	z	0
15	MOTA	2062	O3BAANP Z 379	13.854	56.738	17.611	0.50 47.44	Z	0
	ATOM	2063	O3BBANP Z 379 PA AANP Z 379	16.375 17.533	57.916	20.971 17.115	0.50 53.88 0.50 51.30	Z Z	P
	ATOM ATOM	2064 2065	PA AANP Z 379 PA BANP Z 379	18.302	56.644 56.815	17.115	0.50 51.30	z	P
	ATOM	2066	Olaaanp z 379	18.137	56.443	15.785	0.50 52.19	ž	ô
20	ATOM	2067	Olabanp Z 379	17.740	56.898	16.602	0.50 51.27	z	ō
	ATOM	2068	OZAAANP Z 379	18.354	57.484	18.041	0.50 51.52	z	0
	ATOM	2069	OZABANP Z 379	19.779	56.935	18.073	0.50 51.64	\mathbf{z}	0
	ATOM	2070	O3AAANP Z 379	16.105	57.302	16.924	0.50 51.44	\mathbf{z}	0
05	MOTA	2071	O3ABANP Z 379	17.600	57.938	18.878	0.50 50.89	z	0
25	MOTA	2072	O5*AANP Z 379 O5*BANP Z 379	17.177 17.867	55.295 55.497	17.877 18.751	0.50 50.92 0.50 47.15	z	0
	ATOM	2074	C5*AANP Z 379	17.877	54.090	17.490	0.50 47.94	z	č
	ATOM	2075	C5*BANP Z 379	17.722	54.257	18.009	0.50 40.88	ž	č
	MOTA	2076	C4*AANP Z 379	17.460	52.862	18.318	0.50 47.92	z	c
30	MOTA	2077	C4*BANP Z 379	17.263	53.099	18.926	0.50 36.96	z	C
	MOTA	2078	04*AANP Z 379	18.576	52.400	19.179	0.50 47.21	z	0
	MOTA	2079	04*BANP Z 379	18.369	52.549	19.752	0.50 33.82	z	0
	MOTA MOTA	2080 2081	C3*AANP Z 379 C3*BANP Z 379	16.328 16.203	53.019 53.417	19.359 20.009	0.50 47.98 0.50 33.98	z	C
35	MOTA	2082	O3*AANP Z 379	15.560	51.846	19.588	0.50 48.47	ž	ŏ
55	ATOM	2083	03*BANP Z 379	15.320	52.350	20.339	0.50 32.96	ž	ŏ
	ATOM	2084	C2*AANP Z 379	17.076	53.566	20.584	0.50 47.21	z	C
	ATOM	2085	C2*BANP Z 379	17.064	53.934	21.164	0.50 32.17	z	C
	ATOM	2086	02*AANP Z 379	16.398	53.519	21.825	0.50 48.99	z	0
40	ATOM	2087	02*BANP Z 379	16.446	54.056	22.437	0.50 30.71	Z	0
	ATOM	2088 2089	C1*AANP Z 379 C1*BANP Z 379	18.369 18.273	52.807 53.024	20.558	0.50 46.20 0.50 31.00	z	c
	ATOM ATOM	2089	N9 AANP Z 379	19.533	53.632	21.121	0.50 31.00	ž	N
	ATOM	2091	N9 BANP Z 379	19.537	53.738	21.552	0.50 27.84	ž	N
45	ATOM	2092	C8 AANP Z 379	20.137	54.688	20.410	0.50 43.51	z	C
	ATOM	2093	C8 BANP Z 379	20.190	54.721	20.820	0.50 26.21	\mathbf{z}	C
	ATOM	2094	N7 AANP Z 379	21.138	55.258	21.064	0.50 43.16	z	N
	MOTA	2095	N7 BANP Z 379 C5 AANP Z 379	21.273	55.211 54.563	21.389	0.50 27.05 0.50 43.37	Z	C
50	ATOM	2096 2097	C5 AANP Z 379 C5 BANP Z 379	21.222	54.538	22.228 22.561	0.50 43.37 0.50 27.46	z	č
50	ATOM	2098	C6 AANP Z 379	22.077	54.630	23.408	0.50 41.80	z	č
	ATOM	2099	C6 BANP Z 379	22.300	54.555	23.675	0.50 26.76	z	č
	ATOM	2100	N6 AANP Z 379	23.058	55.506	23.571	0.50 41.70	z	N
	ATOM	2101	N6 BANP Z 379	23.356	55.348	23.750	0.50 26.20	z	N
55	ATOM	2102	N1 AANP Z 379	21.858	53.706	24.460	0.50 43.30	Z	N
	ATOM	2103	N1 BANP Z 379	22.075	53.675	24.765	0.50 29.25 0.50 42.75	Z	N
	ATOM ATOM	2104	C2 AANP Z 379 C2 BANP Z 379	20.844	52.746 52.806	24.372 24.765	0.50 42.75 0.50 27.75	z z	c
	ATOM	2105	N3 AANP Z 379	19.992	52.607	23.302	0.50 43.98	ž	N
60	ATOM	2107	N3 BANP Z 379	20.052	52.720	23.761	0.50 28.35	z	N
	ATOM	2108	C4 AANP Z 379	20.223	53.538	22.258	0.50 43.59	z	c
	ATOM	2109	C4 BANP Z 379	20.292	53.604	22.682	0.50 27.97	Z	C
	ATOM	2110	P1 FRA Z 379	26.094	48.843	31.713	1.00 52.95	Z	P
15	ATOM	2111	02 FRA Z 379	27.446	48.301	31.747	1.00 53.45	Z Z	0
65	ATOM ATOM	2112	03 FRA Z 379 04 FRA Z 379	25.842 25.079	49.670 47.640	32.927 31.660	1.00 57.52 1.00 53.32	z	0
	ATOM	2113	05 FRA Z 379	25.079	49.788	30.418	1.00 54.94	z	0
	TER	2115	FRAGZ 1		25.700	Z Z	2.00 54.54	-	-
	ATOM	2116	O HOH W 379	0.331	67.542	23.164	1.00 33.20	W	0
70	ATOM	2117	O HOH W 380	28.844	46.119	11.651	1.00 48.79	W	0
	ATOM	2118	O HOH W 381	23.007	73.689	19.317	1.00 39.02	W	0
	ATOM	2119	О НОН W 382	10.568	41.141	28.154	1.00 49.97	W	0

						-41-				
	ATOM	2120	0	HOH W 383	12.722	71.913	24.732	1.00 38.33	W	0
	ATOM	2121	0	HOH W 384	27.119	63.991	29.594	1.00 34.78	W	0
	ATOM	2122	0	HOH W 385	25.822	60.889	31.761	1.00 35.64	W	0
_	ATOM	2123	0	нон w 386	12.649	51.436	29.438	1.00 30.54	W	0
5	ATOM	2124	0	HOH W 387	-1.136	77.886	32.084	1.00 58.06	W	0
	ATOM	2125	0	HOH W 388	-5.994	68.177	27.794	1.00 32.43	W	0
	ATOM ATOM	2126 2127	0	HOH W 389 HOH W 390	30.025 -3.566	50.004 81.854	9.061 26.459	1.00 46.99 1.00 55.28	W	ö
	ATOM	2128	0	HOH W 391	30.646	47.521	34.093	1.00 60.01	W	ö
10	ATOM	2129	ŏ	HOH W 392	-1.097	85.911	26.783	1.00 47.89	w	ŏ
10	ATOM	2130	ŏ	HOH W 393	0.595	65.227	46.406	1.00 53.88	W	ŏ
	ATOM	2131	ŏ	HOH W 394	6.207	71.002	50.031	1.00 52.47	W	ō
	ATOM	2132	o	HOH W 395		. 55.170	38.782	1.00 41.90	W	0
	ATOM	2133	0	HOH W 396	-12.360	69.423	40.011	1.00 62.19	W	0
15	ATOM	2134	0	HOH W 397	10.584	80.817	23.752	1.00 42.95	W	0
	ATOM	2135	0	HOH W 398	20.285	61.152	38.189	1.00 57.76	W	0
	MOTA	2136	0	HOH W 399	38.138	63.320 63.417	28.926 18.017	1.00 63.01 1.00 42.85	W	0
	ATOM	2137 2138	0	HOH W 400 HOH W 401	36.205 10.940	46.826	29.244	1.00 42.85	W	0
20	ATOM	2139	ŏ	HOH W 402	28.740	45.402	31.083	1.00 57.98	W	ő
20	ATOM	2140	ŏ	HOH W 403	16.667	51.609	23.943	1.00 49.28	w	ŏ
	ATOM	2141	ŏ	HOH W 404	0.650	83.566	28.516	1.00 48.67	W	ō
	ATOM	2142	ō	HOH W 405	23.052	81.277	32.597	1.00 79.68	W	0
	ATOM	2143	0	HOH W 406	21.015	66.488	25.190	1.00 51.11	W	0
25	ATOM	2144	0	HOH W 407	29.555	78.569	17.681	1.00 72.97	W	0
	ATOM	2145	0	HOH W 408	23.196	68.069	19.434	1.00 38.38	W	0
	ATOM	2146	0	HOH W 409	-7.313	65.296	29.334	1.00 66.68	M	0
	MOTA	2147 2148	0	HOH W 410 HOH W 411	24.377 18.676	54.450 56.503	33.733 40.201	1.00 39.04 1.00 43.61	M	ö
30	ATOM ATOM	2148	ö	HOH W 411	19.799	63.234	10.818	1.00 60.37	W	ő
50	MOTA	2150	ŏ	HOH W 413	4.227	81.623	22.473	1.00 45.07	w	ŏ
	ATOM	2151	ŏ	HOH W 414	35.586	63.256	25.029	1.00 58.40	W	ō
	ATOM	2152	ō	HOH W 415	26.042	47.904	6.604	1.00 63.98	W	0
	ATOM	2153	0	HOH W 416	0.125	61.540	20.664	1.00 58.49	W	0
35	ATOM	2154	0	HOH W 417	15.750	58.426	38.595	1.00 51.37	W	0
	ATOM	2155	0	HOH W 418	8.114	48.760	24.263	1.00 66.46	W	0
	ATOM	2156	0	HOH W 419	-13.534	60.538	36.389	1.00 56.48 1.00 56.53	W	0
	ATOM	2157 2158	0	HOH W 420 HOH W 421	37.492 11.597	60.906 49.198	4.499	1.00 56.53 1.00 55.46	W	0
40	ATOM	2159	o	HOH W 421	29.535	40.480	27.301	1.00 39.07	W	ŏ
-10	ATOM	2160	ŏ	HOH W 423	-9.419	60.202	32.744	1.00 49.49	W	ō
	ATOM	2161	ō	HOH W 424	-3.387	80.285	33.001	1.00 53.18	W	0
	ATOM	2162	0	HOH W 425	22.854	68.702	38.913	1.00 56.31	W	0
	ATOM	2163	0	HOH W 426	5.516	90.168	27.801	1.00 57.26	W	0
45	ATOM	2164	0	HOH W 427	42.341	62.424	13.295	1.00 70.57	W	0
	ATOM	2165	0	HOH W 428 HOH W 429	50.104	46.432	21.896 8.236	1.00 59.70 1.00 38.20	W	0
	ATOM ATOM	2166 2167	0	HOH W 429	19.133 14.218	50.530 90.460	15.295	1.00 59.43	W	ő
	ATOM	2168	ö	HOH W 431	20.996	76.724	18.128	1.00 68.02	w	ő
50	ATOM	2169	ŏ	HOH W 432	28.748	65.408	11.519	1.00 55.89	W	ō
	ATOM	2170	ō	HOH W 433	33.109	52.617	3.045	1.00 66.13	W	0
	MOTA	2171	0	HOH W 434	-0.097	51.530	27.181	1.00 62.48	W	0
	MOTA	2172	0	HOH W 435	34.328	49.913	33.453	1.00 80.02	W	0
	MOTA	2173	0	HOH W 436	16.321	46.597	36.609	1.00 55.74	M	0
55	ATOM	2174	0	HOH W 437	15.506	88.823 68.090	36.550 36.659	1.00 60.31 1.00 43.23	W	0
	ATOM ATOM	2175 2176	0	HOH W 438 HOH W 439	-10.288 35.236	49.316	7.956	1.00 47.01	W	ö
	ATOM	2177	Ö	HOH W 440	-2.382	64.267	14.669	1.00 54.31	w	ŏ
	ATOM	2178	ŏ	HOH W 441	3.145	71.184	22.878	1.00 32.15	W	ŏ
60	ATOM	2179	ŏ	HOH W 442	13.920	51.205	25.014	1.00 47.83	W	0
	ATOM	2180	0	HOH W 443	-0.162	59.596	37.808	1.00 46.99	W	0
	ATOM	2181	0	HOH W 444	21.993	67.937	15.891	1.00 41.38	W	0
	ATOM	2182	0	HOH W 445	18.406	49.826	26.693	1.00 48.92	W	0
-	ATOM	2183	0	HOH W 446	27.317	49.713	35.324	1.00 50.93	W	0
65	MOTA	2184	0	HOH W 447	32.044	55.554	32.480	1.00 59.20 1.00 66.60	W	0
	MOTA	2185 2186	0	HOH W 448 HOH W 449	15.585 28.577	66.847 85.371	22.965 20.089	1.00 66.60	W	0
	ATOM	2187	0	HOH W 450	19.255	74.406	43.569	1.00 78.23	W	ő
	ATOM	2188	ő	HOH W 451	46.877	44.566	20.648	1.00 63.82	w	0
70	ATOM	2189	ō	HOH W 452	18.724	77.353	37.945	1.00 74.74	W	0
	ATOM	2190	0	HOH W 453	32.145	68.599	9.155	1.00 80.54	W	0
	ATOM	2191	0	HOH W 454	4.355	81.219	35.183	1.00 34.92	W	0

						40				
	ATOM	2192	0	HOH W 455	25.635	-42- 56.901	34.614	1.00 47.34	w	0
	ATOM	2192	0	HOH W 455	42.338	49.434	11.100	1.00 72.43	W	ō
	ATOM	2194	ŏ	HOH W 457	~2.051	65.103	18.494	1.00 39.83	W	0
	ATOM	2195	0	HOH W 458	-9.591	72.598	44.168	1.00 64.69	W	0
5	MOTA	2196	0	HOH W 459	20.373	46.614 55.516	27.914 18.515	1.00 38.68 1.00 58.39	w	0
	ATOM ATOM	2197 2198	0	HOH W 460 HOH W 461	0.659 21.076	80.510	26.713	1.00 61.17	W	ŏ
	ATOM	2199	0	HOH W 462	32.155	47.583	8.094	1.00 70.56	W	0
	ATOM	2200	ŏ	HOH W 463	4.044	58.878	44.996	1.00 51.08	W	0
10	ATOM	2201	0	HOH W 464	41.005	53.749	30.770	1.00 75.59	W	0
	MOTA	2202	0	HOH W 465	26.371 18.683	63.533 73.320	-4.679 26.848	1.00 74.46 1.00 53.79	W	0
	ATOM	2203	0	HOH W 466 HOH W 467	31.520	71.009	32.011	1.00 56.96	W	ŏ
	ATOM	2205	ŏ	HOH W 468	17.101	44.021	28.295	1.00 65.42	W	0
15	ATOM	2206	ō	HOH W 469	39.280	50.487	10.873	1.00 71.08	W	0
	ATOM	2207	0	HOH W 470	37.290	42.352	23.513	1.00 70.13	W	0
	ATOM	2208	0	HOH W 471 HOH W 472	5.578 7.437	77.441 83.010	49.897 37.688	1.00 69.56 1.00 69.84	W	ő
	ATOM	2209 2210	0	HOH W 473	26.352	64.806	24.911	1.00 54.06	w	ō
20	ATOM	2211	ŏ	HOH W 474	11.127	50.403	42.491	1.00 74.19	W	0
	MOTA	2212	0	HOH W 475	13.078	66.605	47.781	1.00 64.41	W	0
	MOTA	2213	0	HOH W 476	33.069	47.485	4.075	1.00 73.62 1.00 60.28	W	0
	ATOM	2214	0	HOH W 477 HOH W 478	16.310 10.526	47.636 56.684	48.949	1.00 65.54	W	ŏ
25	ATOM	2215	ŏ	HOH W 479	8.120	87.653	17.142	1.00 54.25	W	0
	ATOM	2217	ŏ	HOH W 480	8.395	84.399	35.638	1.00 53.58	W	0
	MOTA	2218	0	HOH W 481	37.470	55.653	9.464	1.00 46.07	W	0
	ATOM	2219	0	HOH W 482 HOH W 483	26.702 45.743	61.295 51.322	39.749	1.00 63.14 1.00 64.82	W	ö
30	ATOM ATOM	2220 2221	0	HOH W 483 HOH W 484	26.243	53.676	32.375	1.00 76.35	w	ŏ
50	ATOM	2222	ŏ	HOH W 485	28.613	53.324	28.097	1.00 38.88	W	0
	ATOM	2223	0	HOH W 486	4.244	65.989	13.927	1.00 36.47	W	0
	ATOM	2224	0	HOH W 487	24.103	54.829 64.104	31.073 14.517	1.00 48.23 1.00 46.59	W	0
35	ATOM	2225 2226	0	HOH W 488 HOH W 489	16.440 37.058	53.211	10.107	1.00 41.19	W	ő
33	ATOM	2227	ŏ	HOH W 490	1.626	58.930	43.465	1.00 56.15	W	0
	ATOM	2228	0	HOH W 491	5.404	80.824	37.937	1.00 49.30	W	0
	ATOM	2229	0	HOH W 492	3.696	83.191	19.871	1.00 55.84	W	0
40	MOTA	2230 2231	0	HOH W 493 HOH W 494	9.216 36.460	69.339 55.040	23.781 25.386	1.00 49.12	W	ő
40	ATOM	2232	ŏ	HOH W 495	29.035	64.618	25.993	1.00 44.19	W	ō
	ATOM	2233	ŏ	HOH W 496	-1.211	81.253	28.481	1.00 49.42	W	0
	ATOM	2234	0	HOH W 497	-13.349	74.056	40.995	1.00 57.64 1.00 54.51	W	0
45	ATOM	2235 2236	0	HOH W 498 HOH W 499	22.952 8.061	75.394 54.650	20.894 41.586	1.00 54.51 1.00 49.70	W	ö
43	ATOM ATOM	2237	0	HOH W 500	-4.078	73.918	41.599	1.00 51.57	W	ō
	ATOM	2238	ŏ	HOH W 501	26.284	56.747	2.127	1.00 52.08	W	0
	MOTA	2239	0	HOH W 502	30.005	48.619	30.666	1.00 72.19	W	0
50	MOTA	2240	0	HOH W 503 HOH W 504	20.159 -5.361	65.366 63.850	13.420 28.736	1.00 51.24 1.00 60.73	w	ö
50	ATOM	2241 2242	0	HOH W 505	26.955	52.505	30.145	1.00 52.17	W	ō
	ATOM	2243	ŏ	HOH W 506	0.745	55.925	28.349	1.00 47.50	W	0
	ATOM	2244	0	HOH W 507	13.465	63.276	17.023	1.00 63.56	W	0
	ATOM	2245	0	HOH W 508 HOH W 509	-0.920 -8.382	64.629 72.769	40.572 39.661	1.00 40.57 1.00 58.85	W	ö
55	MOTA	2246	0	HOH W 509 HOH W 510	19.488	70.756	41.864	1.00 49.15	W	ŏ
	MOTA	2248	ŏ	HOH W 511	14.101	54.714	36.057	1.00 57.27	W	0
	ATOM	2249	0	HOH W 512	31.885	61.378	38.523	1.00 62.27	W	0
	ATOM	2250	0	HOH W 513	35.755	51.839	8.257 25.470	1.00 47.13	W	0
60	ATOM	2251 2252	0	HOH W 514 HOH W 515	17.069 -4.640	82.457 64.734	26.208	1.00 35.90	W	ŏ
	ATOM	2253	Ö	HOH W 516	28.342	79.720	28.289	1.00 51.97	W	0
	MOTA	2254	0	HOH W 517	28.930	63.693	33.886	1.00 47.21	W	0
	MOTA	2255	0	HOH W 518	14.019	51.336	17.356	1.00 74.59	w	0
65	ATOM	2256 2257	0	HOH W 519 HOH W 520	16.446 32.520	79.651 63.699	42.696 25.738	1.00 57.23	w	Ö
	ATOM	2257	0	HOH W 521	-11.168	62.126	35.907	1.00 65.36	w	ŏ
	ATOM	2259	ŏ	HOH W 522	13.702	76.196	48.300	1.00 61.59	W	0
	ATOM	2260	0	HOH W 523	1.241	58.718	25.331	1.00 64.44	W	0
70		2261	0	HOH W 524 HOH W 525	14.477 12.372	78.178 54.887	21.588 20.646	1.00 64.83	W	0
	MOTA	2262 2263	0	HOH W 525	7.266	74.256	14.263	1.00 39.73	W	ő
	MION	2203	_							

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	ATOM	2264	0	HOH W	527	20.091	44.006	35.105	1.00 50.82	W	0
	ATOM	2265	Ó	HOH W	528	1.165	69.375	46.475	1.00 57.89	W	0
	ATOM	2266	0	HOH W	529	19.142	46.127	35.660	1.00 45.19	₩	0
	ATOM	2267	0	HOH W	530	42.086	55.304	19.791	1.00 71.79	W	0
5	ATOM	2268	0	HOH W	531	25.087	50.111	39.148	1.00 63.76	W	0
	ATOM	2269	0	HOH W	532	5.318	61.373	18.508	1.00 62.59	W	0
	ATOM	2270	0	HOH W	533	29.675	78.586	23.627	1.00 58.56	W	0
	ATOM	2271	0	HOH W	534	19.557	76.701	12.869	1.00 68.72	W	0
	ATOM	2272	0	HOH W	535	42.115	57.119	21.522	1.00 71.32	W	0
10	ATOM	2273	О	HOH W	536	0.634	77.003	19.831	1.00100.00	₩	0
	ATOM	2274	0	HOH W	537	19.709	88.994	42.992	1.00 58.23	W	0
	ATOM	2275	0	HOH W	538	13.524	50.624	47.508	1.00 75.63	W	0
	ATOM	2276	0	HOH W	539	11.617	86.001	30.094	1.00 68.80	₩	0
	ATOM	2277	0	HOH W		-7.680	59.135	43.088	1.00 61.92	W	0
15	TER	2278		HOH W						W	
	ATOM	2279	C1	FRA V		18.019	80.374	32.848	1.00 57.37	v	С
	ATOM	2280	C2	FRA V		17.378	79.416	33.865	1.00 55.67	v	C
	ATOM	2281	C3	fra v		17.724	79.837	35.320	1.00 57.54	v	C
	ATOM	2282	04	FRA V		17.702	79.994	31.523	1.00 54.83	v	0
20	ATOM	2283	05	FRA V		15.964	79.445	33.671	1.00 53.75	v	0
	ATOM	2284	06	FRA V	541	16.818	79.285	36.284	1.00 58.10	v	0
	ATOM	2285	0	HOH V		21.116	58.251	20.758	1.00 34.64	v	0
	TER	2286		нон у	2					v	

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-44-

Table 2 – coordinates for the two molecules in the asymmetric unit of [T287] Aurora A

(122-396) in complex with an inhibitor of formula II in space group P2₁

```
5 REMARK [No title given]
    REMARK [No title given]
    REMARK [No title given]
    REMARK Aurora complex with M535136. Refined structure. Solved by
   REMARK molecular replacement using a partly refined aurora structure
10 REMARK from the trigonal crystal form. Original MR model derived
REMARK from a PKA alignment. Inhibitor occupies much of active site
    REMARK cleft and usual interactions at adenine site. Superposition
   REMARK with FKA shows a very wide, open active site cleft.
REMARK coordinates from restrained individual B-factor refinement
15 REMARK refinement resolution: 500.0 - 2.1 A
    REMARK starting r= 0.2306 free_r= 0.2716
    REMARK final
                      r= 0.2256 free_r= 0.2677
REMARK B rmsd for bonded mainchain atoms= 1.521 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 2.205 target= 2.0
20 REMARK B rmsd for angle mainchain atoms= 2.492 target= 2.0
    REMARK B rmsd for angle sidechain atoms= 3.350 target= 2.5
    REMARK rweight= 0.1000 (with wa= 3.00741)
    REMARK target= mlf steps= 30
    REMARK sg= P2(1)a= 52.603 b= 88.421 c= 67.832 alpha=90 beta= 90.013 gamma= 90
25 REMARK parameter file 1 : MSI_CNX_TOPPAR:protein_rep.param
    REMARK parameter file 2 : fra.par
REMARK parameter file 3 : MSI_CNX_TOPPAR:water_rep.param
    REMARK molecular structure file: reb9.mtf
    REMARK input coordinates: anneal_reb_1.pdb
30 REMARK reflection file= aurora-p21.cv
    REMARK ncs= none
    REMARK B-correction resolution: 6.0 - 2.1
    REMARK initial B-factor correction applied to fobs :
    REMARK B1= 1.629 B22= -1.218 B33= -0.411
REMARK B12= 0.000 B13= 0.000 B23= 0.000
35 REMARK
    REMARK B-factor correction applied to coordinate array B: -0.233
    REMARK bulk solvent: (Mask)density level= 0.31769 e/A^3, B-factor=51.8227 A^2
    REMARK reflections with | Fobs | /sigma_F < 0.0 rejected REMARK reflections with | Fobs | > 10000 * rms (Fobs) rejected
40 REMARK theoretical total number of refl. in resol. range:
                                                                               36279(100.0 %)
    REMARK number of unobserved reflections (no entry or |F|=0):
                                                                               9992 (27.5 % )
    REMARK number of reflections rejected:
                                                                                   0 (0.0%)
                                                                               26287 (72.5 % )
    REMARK total number of reflections used:
                                                                               25018 (69.0 % )
    REMARK number of reflections in working set:
45 REMARK number of reflections in test set:
                                                                                 1269 ( 3.5 % )
    REMARK FILENAME="bindividual.pdb"
    REMARK DATE: Feb-12-2001 13:11:17
                                                    created by user: mar345
    REMARK Written by CNX VERSION:2000.1
CRYST1 52.603 88.421 67.832 90.00 90.01 90.00 P 1 21 1
                  0.019010 0.000000 0.000003
50 SCALE1
                                                             0.00000
    SCALE2
                  0.000000 0.011310 0.000000
                                                             0.00000
    SCALES
                  0.000000 0.000000 0.014742
                                                              0.00000
                                          32.162 112.290 73.232 1.00 49.44
    MOTA
                1 CB GLN A 126
               2 CG GLN A 126
                                          32.015 113.484 72.284 1.00 51.02
    MOTA
                                          32.563 113.219 70.887 1.00 51.57
31.961 112.499 70.089 1.00 51.89
55 ATOM
               3 CD GLN A 126
               4 OE1 GLN A 126
    MOTA
                                         33.717 113.803 70.589 1.00 52.45
31.499 110.010 73.975 1.00 46.32
31.745 110.223 75.161 1.00 48.00
    мота
               5 NE2 GLN A 126
               6 C GLN A 126
7 O GLN A 126
    MOTA
                                                                                                  C
    MOTA
               8 N GLN A 126
                                          29.765 111.655 73.328 1.00 47.98
60 ATOM
                                           31.143 111.162 73.040 1.00 47.45
31.523 108.792 73.443 1.00 43.51
    ATOM
                9 CA GLN A 126
              10 N TRP A 127
    A TOM
                                          31.864 107.618 74.238 1.00 40.38
30.998 106.418 73.836 1.00 40.28
    ATOM
              11 CA TRP A 127
               12 CB TRP A 127
    ATOM
                                          30.998 106.418 73.836 1.00 40.28
29.528 106.692 73.786 1.00 37.53
28.575 106.442 74.826 1.00 36.46
27.309 106.835 74.335 1.00 36.39
28.669 105.924 76.123 1.00 34.75
              13 CG TRP A 127
65 ATOM
              14 CD2 TRP A 127
    ATOM
    MOTO
              15 CE2 TRP A 127
    MOTE
              16 CE3 TRP A 127
                                          28.827 107.215 72.740 1.00 37.84
    ATOM
             17 CD1 TRP A 127
```

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	MOTA	18	NE1	TRP A	127	27.490	107.302	73.060	1.00 36.81	A	N
	MOTA	19		TRP A			106.725	75.097	1.00 36.10	A	C
	MOTA	20		TRP A			105.814	76.884	1.00 37.35	A	C
	MOTA	21		TRP A			106.214	76.366	1.00 37.47 1.00 38.84	A A	C
5	ATOM	22 23	c	TRP A		33.329	107.765	74.024 73.117	1.00 37.85	A	Ö
	ATOM	24	N	ALA A			106.349	74.858	1.00 36.22	A	N
	ATOM	25	CA	ALA A			105.891	74.741	1.00 35.97	A	С
	ATOM	26	CB	ALA A		36.136	106.763	75.582	1.00 35.91	A	С
10	MOTA	27	C	ALA A		35.289	104.441	75.200	1.00 35.31	A	С
	ATOM	28	0	ALA A		34.514	104.015	76.056	1.00 34.64	A	0
	MOTA	29	N	LEU A		36.221	103.688	74.626 74.976	1.00 33.98 1.00 34.14	A	N
	ATOM	30 31	CB	LEU A		36.385 37.556	102.283	74.191	1.00 34.14	A A	č
15	ATOM	32	CG	LEU A		37.816	100.175	74.339	1.00 35.39	A	č
	MOTA	33		LEU A		36.514	99.396	74.175	1.00 34.09	A	С
	MOTA	34		LEU A	129	38.841	99.729	73.300	1.00 33.75	A	C
	MOTA	35	C	LEU A			102.092	76.476	1.00 33.77	A	c
20	MOTA	36	0	LEU A			101.182	77.083 77.072	1.00 33.18 1.00 34.08	A	O N
20	MOTA	37 38	N CA	ALA A			102.974 102.918	77.072	1.00 34.08	A	C
	ATOM	38	CB	ALA A	130	38.757	103.954	78.836	1.00 33.52	A	č
	ATOM	40	c	ALA A		36.483	103.112	79.415	1.00 33.70	A	ē
	ATOM	41	ō	ALA A		36.615	103.026	80.633	1.00 35.42	A	0
25	ATOM	42	N	ASP A		35.315	103.380	78.841	1.00 33.03	A	N
	ATOM	43	CA		131	34.092	103.588	79.632	1.00 31.53	A	C
	ATOM	44 45	CB		131 131	33.094 33.415	104.444	78.849 78.898	1.00 35.30	A A	Ċ
	MOTA MOTA	45	OD1		131	32.854	106.665	78.066	1.00 40.43	A	ŏ
30	ATOM	47		ASP A		34.209	106.335	79.770	1.00 39.65	A	0
	MOTA	48	C	ASP A	131	33.404	102.274	79.970	1.00 29.88	A	C
	MOTA	49	0	ASP A		32.510	102.223	80.816	1.00 27.49	A	0
	MOTA	50	N		132	33.836	101.211	79.305	1.00 28.87 1.00 27.75	A	C N
35	MOTA MOTA	51 52	CA	PHE A		33.232 32.617	99.906 99.450	79.487 78.168	1.00 27.75	A A	č
33	ATOM	53	CG	PHE A			100.504	77.478	1.00 24.75	A	č
	MOTA	54		PHE A		30.535	100.808	77.899	1.00 22.62	A	C
	MOTA	55		PHE A		32.356	101.195	76.403	1.00 22.91	A	С
	MOTA	56		PHE A		29.794	101.788	77.249	1.00 26.12	A	C
40	MOTA	57 58	CE2	PHE A		31.626 30.340	102.174	75.749 76.173	1.00 25.55 1.00 23.27	A A	c
	MOTA	59	C	PHE A		34.164	98.801	79.947	1.00 27.73	A	č
	ATOM	60	ŏ	PHE A		35.375	98.852	79.736	1.00 27.55	A	ō
	ATOM	61	N	GLU A	133	33.560	97.798	80.575	1.00 27.29	A	N
45	MOTA	62	CA	GLU A		34.254	96.596	81.004	1.00 26.91	A	c
	ATOM	63	CB	GLU A		33.863	96.187 97.120	82.415 83.506	1.00 29.96 1.00 35.88	A A	C
	ATOM	64 65	CD	GLU A		34.290 33.945	96.546	84.858	1.00 39.31	A	č
	ATOM	66	OE1	GLU A		34.491	95.469	85.189	1.00 40.33	A	ō
50	ATOM	67		GLU A		33.120	97.153	85.576	1.00 40.57	A	0
	MOTA	68	С	GLU A		33.665	95.582	80.034	1.00 24.82	A	С
	MOTA	69	0	GLU A		32.444	95.536	79.854	1.00 21.66	A A	O N
	MOTA	70 71	N CA	ILE A		34.523 34.091	94.787 93.784	79.410 78.443	1.00 22.52	A	C
55	ATOM	72	CB	ILE A		35.115	93.688	77.286	1.00 23.20	A	č
	ATOM	73	CG2	ILE A		34.652	92.704	76.240	1.00 23.57	A	С
	ATOM	74	CG1	ILE A	134	35.317	95.073	76.668	1.00 26.34	A	C
	ATOM	75		ILE A		34.059	95.709	76.121	1.00 27.45	A	C
60	MOTA	76 77	0	ILE A		33.935 34.737	92.413 92.024	79.093 79.941	1.00 23.10 1.00 24.84	A A	c
00	MOTA	78	N	GLY A		32.904	91.679	78.681	1.00 24.78	λ	N
	ATOM	79	CA	GLY A		32.648	90.355	79.231	1.00 22.02	A	c
	ATOM	80	c	GLY A	135	32.677	89.246	78.193	1.00 20.46	A	C
	MOTA	81	0	GLY A		33.404	89.330	77.212	1.00 18.06	A	0
65	MOTA	82	N	ARG A		31.867	88.212	78.391	1.00 23.35 1.00 25.21	A A	N C
	MOTA	83 84	CA	ARG A		31.852 31.078	87.077 85.902	77.464 78.064	1.00 25.21	A A	c
	MOTA	85	CG	ARG A		29.601	86.174	78.284	1.00 28.67	A	c
	MOTA	86	CD	ARG A		28.870	84.914	78.725	1.00 29.20	A	C
70	MOTA	87	NE	ARG A	136	27.497	85.201	79.121	1.00 31.23	A	N
	MOTA	88	CZ	ARG A		26.417	84.687	78.532	1.00 34.58	A A	C
	MOTA	89	NH1	ARG A	136	26.546	83.847	77.512	1.00 33.49	A	N

								-46-						
	ATOM	90	NH2	ARG	A	136	25.204	85.028	78.958	1.00	34.12	2	A	N
	ATOM	91	С	ARG			31.285	87.369	76.084		26.22	1	Ā	C
	ATOM	92	0	ARG			30.450	88.260	75.916		24.47	2		0
_	ATOM	93	N	PRO			31.749	86.620	75.070		26.55	2		и.
5	ATOM	94	CD	PRO			32.907	85.714	75.122		27.27	2		c
	ATOM	95 96	CA	PRO			31.285 32.236	86.786 85.898	73.690 72.887		26.49	2		c
	ATOM	97	CG	PRO		137	33.477	85.858	73.729		25.14	1		č
	ATOM	98	c	PRO			29.856	86.276	73.609		27.01		Š.	č
10	MOTA	99	ò	PRO	Α	137	29.538	85.226	74.169	1.00	26.92	2	A	0
	ATOM	100	N	LEU			28.995	87.018	72.924		27.88	2		N
	MOTA	101	CA	LEU			27.602	86.615	72.779	1.00	29.09		A.	c
	ATOM	102 103	CB	LEU		138 138	26.691 26.450	87.843 88.473	72.865 74.240		27.78 26.22	2		C
15	ATOM	103	CG	LEU			27.758	88.636	74.240		29.17	- 2		Ċ
13	ATOM	105		LEU			25.771	89.816	74.075		20.07		À	· c
	ATOM	106	C	LEU		138	27.403	85.907	71.438		30.81		Ā	Ċ
	ATOM	107	0	LEU	Α	138	26.619	84.964	71.329		32.24		A	0
	ATOM	108	N	GLY		139	28.124	86.367	70.424		32.34		A	N
20	ATOM	109	CA	GLY			28.014	85.773	69.109	1.00			A.	C
	MOTA	110 111	C	GLY		139	29.136 29.859	86.215 87.166	68.190 68.488		38.07	- 4	A.	C
	ATOM	112	N	LYS			29.281	85.519	67.066		41.32		À	N
	ATOM	113	CA	LYS			30.320	85.831	66.092		43.10	- 3		c
25	ATOM	114	CB	LYS	A	140	31.244	84.633	65.917	1.00	44.15	1	A	C
	ATOM	115	C	LYS			29.703	86.216	64.751		44.25		A	C
	ATOM	116	0	LYS			28.615	85.755	64.403		43.38		A.	0
	ATOM	117 118	N CA	GLY			30.406 29.939	87.066 87.527	64.007 62.705		45.98 47.85		A. A.	N
30	ATOM	119	CB	GLY			29.270	88.895	62.842		49.28		n.	č
50	ATOM	120	c	GLY			31.109	87.613	61.731		48.68		Ā	č
	ATOM	121	ŏ	GLY			32.235	87.245	62.073	1.00	48.92		A	0
	ATOM	122	N	ALA			30.842	88.111	60.525	1.00	48.78		A	N
0.5	ATOM	123	CA	ALA			31.877	88.226	59.502	1.00	47.65		A.	C
35	MOTA	124 125	CB	ALA			31.247 32.730	88.156 89.488	58.115 59.620		48.08 46.86		A. A.	C
	MOTA	126	ŏ	ALA			33.828	89.550	59.063		46.94		A.	ŏ
	ATOM	127	N	PHE			32.242	90.492	60.343		45.34		Ą	N
	MOTA	128	CA	PHE			33.004	91.731	60.477		43.93		A	C
40	MOTA	129	CB	PHE			32.193	92.907	59.920		43.56		Ą	C
	ATOM	130	CG	PHE			31.628	92.653	58.550 58.397		43.95 44.56		A	C
	MOTA	131 132		PHE			30.352 32.385	92.118 92.915	57.413		44.21		A. A.	c
	ATOM	133		PHE			29.836	91.845	57.129		44.68		A	č
45	ATOM	134		PHE			31.881	92.645	56.141		44.72		A	С
	ATOM	135	CZ	PHE			30.604	92.109	55.999		44.72		A	C
	ATOM	136	C	PHE			33.456	92.045	61.901		42.13		A	c
	MOTA	137 138	0	PHE			34.137 33.085	93.043 91.183	62.132 62.846		41.48		A.	O
50	ATOM ATOM	139	N CA	GLY			33.452	91.396	64.235		37.57		A.	Č
-	ATOM	140	č	GLY			32.537	90.631	65.171		36.23		A	č
	ATOM	141	0	GLY			31.625	89.938	64.721		35.58		A	0
	ATOM	142	N	ASN			32.763	90.763	66.474		34.55		A	N
	ATOM	143	CA	ASN			31.947	90.052	67.453		32.65		A	C
55	ATOM	144 145	CB	ASN ASN			32.842 33.913	89.187 88.458	68.341 67.549		34.14		A A	c
	ATOM	146		ASN			35.068	88.893	67.489		36.74		A	õ
	ATOM	147		ASN			33.531	87.352	66.924		35.73		A	N
	ATOM	148	C	ASN			31.096	90.959	68.331		30.37		A	C
60	ATOM	149	0	ASN			31.232	92.183	68.308	1.00	31.36		A	0
	ATOM	150	N	VAL			30.214	90.337	69.107		27.53		A	N
	ATOM	151 152	CA	VAL		146	29.326 27.836	91.051 90.769	70.013 69.684	1.00	24.74 26.28		A A	C
	ATOM	153	CG1				26.932	91.644	70.548	1.00	24.90		A.	č
65	ATOM	154	CG2				27.573	91.006	68.211	1.00	28.46		A	C
	MOTA	155	C	VAL	A	146	29.605	90.546	71.424		22.82		A	C
	ATOM	156	0	VAL			29.599	89.341	71.660		24.33		A.	0
	ATOM	157 158	N CA	TYR			29.836 30.125	91.461 91.081	72.357 73.738		20.11 18.69		A A	N
70		159	CB	TYR			31.530	91.523	74.145		16.30		A.	č
	ATOM	160	CG	TYR			32.646	91.083	73.231		20.13		A	č
	ATOM	161	CD1			147	32.849	91.701	71.997		19.62		A	C

							-47-				
	ATOM	162	CE1	TYR A	147	33.898	91.318	71.162	1.00 22.76	A	C
	ATOM	163		TYR F		33.519	90.059	73.610	1.00 19.37	A	С
	MOTA	164	CE2	TYR Z	147	34.574	89.661	72.777	1.00 20.22	A	С
	ATOM	165	CZ	TYR A		34.755	90.298	71.559	1.00 23.88	A	c
5	ATOM	166	OH	TYR I		35.788	89.925	70.727	1.00 27.07	A	0
	ATOM	167	C	TYR 2		29.177	91.690 92.731	74.757 74.521	1.00 17.31 1.00 16.25	A A	0
	MOTA	168 169	O N	TYR A		28.568 29.071	91.026	75.903	1.00 17.91	A	N
	MOTA MOTA	170	CA	LEU 2		28.283	91.544	76.996	1.00 16.28	A	c
10	ATOM	171	CB	LEU 2		28.040	90.472	78.054	1.00 19.47	A	c
10	ATOM	172	CG	LEU A		27.148	90.939	79.205	1.00 19.54	A	C
	MOTA	173		LEU A	148	25.844	90.198	79.117	1.00 23.07	A	C
	MOTA	174	CD2	LEU 2		27.809	90.695	80.561	1.00 21.88	A	C
	ATOM	175	С	LEU 2		29.230	92.599	77.555	1.00 16.81	A	c
15	MOTA	176	0	LEU 2		30.449	92.387	77.604 77.962	1.00 17.66 1.00 17.06	A A	N
	MOTA	177	N CA	ALA A	A 149	28.693 29.529	93.740 94.794	78.504	1.00 17.00	A	C
	ATOM ATOM	178 179	CB	ALA I		29.953	95.744	77.400	1.00 16.74	A	č
	MOTA	180	C		A 149	28.778	95.540	79.591	1.00 19.32	A	č
20	ATOM	181	ŏ		149	27.585	95.302	79.815	1.00 17.25	A	0
	MOTA	182	N	ARG :	A 150	29.483	96.442	80.262	1.00 18.18	A	N
	MOTA	183	CA		A 150	28.903	97.215	81.338	1.00 20.87	A	C
	ATOM	184	CB		A 150	29.073	96.435	82.651	1.00 24.33	A A	C
0.5	ATOM	185	CG		A 150	28.543	97.119 96.096	83.890 84.995	1.00 30.19	A	c
25	ATOM	186 187	CD		A 150 A 150	28.265 29.370	95.162	85.167	1.00 33.70	A	N
	ATOM	188	CZ		A 150	29.308		85.897	1.00 35.11	A	c
	ATOM	189	NH1		A 150	28.186	93.735	86.533	1.00 36.02	A	N
	ATOM	190	NH2		A 150	30.365	93.252	85.983	1.00 32.01	A	N
30	ATOM	191	С	ARG .	A 150	29.593	98.574	81.422	1.00 22.84	A	C
	MOTA	192	0		A 150	30.808		81.180	1.00 18.77	A	0
	MOTA	193	N		A 151	28.819		81.727 81.874	1.00 23.89 1.00 26.53	A A	И
	MOTA	194 195	CA		A 151 A 151	29.383	100.958	81.883	1.00 26.52	A	č
35	ATOM	195	CG		A 151	27.420	102.099	80.629	1.00 28.40	A	č
33	ATOM	197	CD		A 151		103.198	80.704	1.00 29.97	A	C
	ATOM	198	OE1		A 151		103.337	81.765	1.00 29.43	A	0
	ATOM	199	OE2		A 151		103.917	79.704	1.00 31.53	A	0
	MOTA	200	С		A 151		100.897	83.242	1.00 27.68	A	C
40	MOTA	201	0		A 151		100.577	84.230 83.288	1.00 28.40 1.00 30.73	A A	N
	MOTA	202	N CA	LYS			101.195	84.523	1.00 33.53	Ā	c
	ATOM	203	CB	LYS			101.691	84.288	1.00 34.64	A	č
	ATOM	205	CG	LYS			100.758	83.531	1.00 37.25	A	С
45	MOTA	206	CD		A 152	35.836	101.367	83.353	1.00 39.94	A	С
	ATOM	207	CE		A 152		100.408	82.629	1.00 40.54	A	С
	MOTA	208	NZ	LYS			101.012	82.399	1.00 41.98 1.00 33.54	A A	N C
	ATOM	209	C		A 152		101.842	85.727 86.790	1.00 35.42	A	Ö
50	ATOM	210 211	N	GLN	A 152 A 153		103.117	85.564	1.00 33.42	A	N
50	ATOM	212	CA		A 153		103.904	86.655	1.00 34.22	A	C
	ATOM	213	CB		A 153	30.568	105.370	86.231	1.00 36.43	A	C
	MOTA	214	CG		A 153		105.975	85.797	1.00 39.77	A	C
	MOTA	215	CD		A 153	32.954		86.889	1.00 42.68	A	C
55	MOTA	216	OE1		A 153	34.107		86.657 88.082	1.00 46.22 1.00 43.83	A	O
	MOTA	217 218	NE2		A 153 A 153	29.316	105.503	87.182	1.00 43.83	A	Č
	ATOM	218	C		A 153		102.938	88.314	1.00 34.62	Ä	ŏ
	ATOM	220	N	SER			103.555	86.371	1.00 32.03	A	N
60	ATOM	221	CA		A 154		103.156	86.794	1.00 29.99	A	C
	ATOM	222	CB		A 154		103.831	85.914	1.00 29.69	A	C
	MOTA	223	OG		A 154		103.510	84.551	1.00 29.28	A	0
	MOTA	224	C		A 154		101.657	86.845 87.398	1.00 29.81 1.00 29.38	A A	0
65	MOTA	225 226	O N		A 154 A 155	25.646	5 101.236 5 100.855	86.261	1.00 29.05	A	N
63	ATOM	226	CA		A 155	27.389		86.276	1.00 30.67	A	č
	ATOM	228	CB		A 155	27.185		87.725	1.00 32.82	A	C
	ATOM	229	CG	LYS	A 155	27.059	97.435	87.912	1.00 39.02	A	C
	ATOM	230	CD	LYS	A 155	26.67		89.342	1.00 43.54	A	C
70		231	CE		A 155	25.20		89.669	1.00 47.18	A	C
	ATOM	232	NZ		A 155	24.902		89.800 85.398	1.00 49.30 1.00 28.46	A A	C
	MOTA	233	С	LYS	A 155	20.22	90.913	65.596	1.00 20.40	Α.	

							-48-				
	MOTA	234	0	LYS F	155	25.706	97.812	85.590	1.00 27.89	A	0
	ATOM	235	N	PHE A		25.831	99.727	84.424	1.00 26.49	A	N
	MOTA	236	CA	PHE A		24.716	99.403	83.536	1.00 23.82	A	C
	MOTA	237	CB	PHE F		24.185	100.698	82.905	1.00 24.31	A	С
5	MOTA	238	CG	PHE A		23.043	100.492	81.955	1.00 24.97 1.00 24.81	A A	C
	ATOM ATOM	239 240	CD1	PHE A	156	21.771 23.244	100.187 100.592	82.428 80.580	1.00 24.81	A	c
	ATOM	241		PHE F		20.705	99.982	81.537	1.00 27.89	A	č
	ATOM	242		PHE F		22.195	100.390	79.685	1.00 24.55	A	č
10		243	CZ	PHE A		20.920	100.084	80.163	1.00 25.32	A	C
	MOTA	244	С	PHE A		25.082	98.381	82.445	1.00 21.90	A	C
	MOTA	245	0	PHE A		26.019	98.582	81.676	1.00 21.26	A	0
	ATOM	246	N	ILE A		24.321	97.294	82.388	1.00 19.42	A A	N
15	MOTA	247	CA	ILE A		24.535 23.863	96.219 94.906	81.418 81.878	1.00 19.66 1.00 20.30	A	c
13	ATOM	248 249	CB CG2	ILE A		23.931	93.876	80.759	1.00 18.66	A	č
	ATOM	250	CG1			24.541	94.373	83.143	1.00 20.54	A	Ċ
	ATOM	251	CD1			25.994	93.979	82.929	1.00 23.70	A	С
	MOTA	252	C	ILE A		23.996	96.515	80.018	1.00 20.08	Α.	С
20	MOTA	253	0		157	22.851	96.955	79.859	1.00 18.61	A .	0
	MOTA	254	N	LEU A		24.819	96.239	79.011	1.00 18.01	A A	N
	ATOM ATOM	255 256	CA CB	LEU A		24.445 24.651	96.436 97.900	77.616 77.220	1.00 19.34 1.00 20.73	A	č
	ATOM	257	CG	LEU 2		25.882	98.644	77.734	1.00 22.83	A	č
25	ATOM	258		LEU A		27.125	98.226	76.965	1.00 23.65	A	c
	ATOM	259	CD2	LEU 2		25.633	100.139	77.576	1.00 24.53	A	С
	ATOM	260	C	LEU A		25.231	95.498	76.688	1.00 19.24	A	С
	MOTA	261	0	LEU 1		25.944	94.623	77.153	1.00 20.32	A	0
20	ATOM	262	N	ALA A		25.077	95.654 94.803	75.379 74.431	1.00 19.56 1.00 19.83	A A	C
30	ATOM ATOM	263 264	CB	ALA A		25.790 24.809	94.009	73.579	1.00 19.54	A	č
	ATOM	265	CB	ALA I		26.673	95.672	73.553	1.00 20.25	A	č
	ATOM	266	ŏ	ALA 2		26.274	96.766	73.143	1.00 19.23	A	0
	ATOM	267	N	LEU 2		27.878	95.190	73.274	1.00 20.17	A	N
35	ATOM	268	CA	PEA 1		28.820	95.944	72.459	1.00 22.21	A	C
	ATOM	269	CB	LEU 2		30.019	96.360	73.326 72.715	1.00 23.33 1.00 27.33	A A	C
	ATOM	270 271	CG CD1		A 160 A 160	31.194 30.789	97.129 98.572	72.410	1.00 27.33	A	č
	ATOM	272	CD2			32.359	97.112	73.699	1.00 26.63	A	č
40	ATOM	273	c	LEU 2		29.298	95.146	71.249	1.00 22.33	A	C
	ATOM	274	0	LEU 2	A 160	29.772	94.021	71.379	1.00 21.48	A	0
	ATOM	275	N	LYS		29.170	95.738	70.067	1.00 23.83	A	N
	ATOM	276	CA	LYS		29.612	95.082	68.840 67.792	1.00 24.70 1.00 24.56	A A	C
45	ATOM	277 278	CB	LYS :	A 161 A 161	28.502 28.735	95.107 94.154	66.635	1.00 26.78	Â	č
45	ATOM	279	CD	LYS		27.431	93.891	65.887	1.00 25.97	A	č
	ATOM	280	CE	LYS		27.612	92.863	64.792	1.00 23.17	A	C
	ATOM	281	NZ	LYS		26.293	92.377	64.315	1.00 22.83	A	N
	ATOM	282	С	LYS :		30.850	95.798	68.314	1.00 25.61	A A	C
50	ATOM	283	0	LYS		30.850 31.907	97.014 95.031	68.146 68.072	1.00 25.29 1.00 27.06	A	O N
	ATOM ATOM	284 285	N CA	VAL :		33.172	95.568	67.585	1.00 28.41	A	č
	ATOM	286	CB	VAL		34.346	95.050	68.456	1.00 31.04	A	č
	ATOM	287	CG1			35.678	95.617	67.957	1.00 31.63	A	C
55	ATOM	288	CG2			34.113	95.427	69.914	1.00 30.41	A	С
	MOTA	289	C		A 162	33.387	95.132	66.139	1.00 28.72	A A	C
	MOTA	290 291	O		A 162 A 163	33.387 33.561	93.942 96.096	65.844 65.241	1.00 28.91 1.00 30.09	A A	N
	ATOM	291	CA		A 163	33.760	95.801	63.823	1.00 31.38	A	č
60	ATOM	293	CB	LEU .		32.670	96.479	62.987	1.00 30.68	A	č
	ATOM	294	CG		A 163	31.207	96.151	63.295	1.00 31.65	A	С
	ATOM	295	CD1		A 163	30.343	97.379	63.035	1.00 33.15	A	С
	MOTA	296	CD2		A 163	30.747	94.985	62.452	1.00 31.46	A	C
65	ATOM ATOM	297 298	. C	LEU .		35.116 35.541	96.333 97.386	63.393 63.865	1.00 32.77 1.00 33.03	A A	0
03	ATOM	298	N	PHE .		35.793	95.610	62.503	1.00 34.61	A	N
	MOTA	300	CA	PHE		37.107	96.043	62.018	1.00 36.93	A	c
	MOTA	301	CB	PHE	A 164	38.068	94.849	61.878	1.00 38.68	A	C
	ATOM	302	CG	PHE .		38.406	94.181	63.180	1.00 40.41	A	C
70	MOTA	303	CD1			37.659		63.639	1.00 41.41	A A	C
	ATOM	304 305		PHE		39.464 37.959		63.960 64.857	1.00 41.14 1.00 41.57	A A	c
	ATOM	305	CEI	PRE .	A 104	37.955	94.489	04.637	1.00 41.37	-	_

							-49-				
	ATOM	306	CE2	PHR 2	164	39.774		65.182	1.00 42.28	A	С
	ATOM	307	cz	PHE A	164	39.020	92.960	65.630	1.00 41.55	A	С
	MOTA	308	C		A 164	37.000	96.759	60.674	1.00 36.27	A	C
5	ATOM ATOM	309	0	PHE I		36.489	96.203 97.993	59.701	1.00 34.52	Α.	. 0
J	ATOM	310 311	N CA	LYS I	A 165 A 165	37.495 37.461	98.809	60.632 59.422	1.00 37.51	A A	N C
	ATOM	312	CB		A 165	38.248		59.635	1.00 39.41	A	c
	ATOM	313	CG	LYS 2		37.700	100.988	60.738	1.00 41.43	A	С
	ATOM	314	CD	LYS 2		38.473		60.820	1.00 43.19	A	C
10	ATOM ATOM	315 316	CE		A 165	37.957		61.941 62.007	1.00 43.06	A A	C
	ATOM	317	C		A 165	38.712 38.016		58.200	1.00 45.01 1.00 39.84	A A	N
	ATOM	318	õ		165	37.332		57.183	1.00 40.35	A	ō
	ATOM	319	N	ALA 2	A 166	39.259	97.629	58.309	1.00 40.50	A	N
15	ATOM	320	CA		A 166	39.930		57.218	1.00 41.24	A	С
	ATOM ATOM	321	CB		A 166 A 166	41.230	96.314	57.717	1.00 40.66 1.00 42.45	A	c
	ATOM	322 323	C		A 166	39.039 39.143	95.850 95.524	55.439	1.00 42.45	A A	C
	ATOM	324	N		A 167	38.160		57.448	1.00 42.58	A	N
20	ATOM	325	CA	GLN A	A 167	37.256	94.255	56.995	1.00 44.47	A	C
	ATOM	326	CB	GLN 3	A 167	36.814	93.405	58.189	1.00 47.08	A	С
	MOTA MOTA	327 328	CD		A 167 A 167	36.076		57.818 58.772	1.00 49.82 1.00 51.86	A	C
	ATOM	329	OE1			36.382 36.182	91.105	59.985	1.00 51.86	A A	0
25	ATOM	330	NE2			36.873	89.880	58.226	1.00 52.20	Ä	N
	ATOM	331	C	GLN A	A 167	36.044	94.856	56.288	1.00 44.78	A	С
	MOTA	332	0		A 167	35.580	94.329	55.277	1.00 44.92	A	0
	ATOM ATOM	333	CA	PEO 1	A 168	35.539	95.965 96.635	56.818 56.232	1.00 45.62 1.00 47.56	A	N
30	ATOM	334 335	CB	LEU I	A 168	34.379 33.899		57.146	1.00 47.56	A A	c
-	ATOM	336	CG		168	33.222		58.476	1.00 43.92	A	č
	ATOM	337	CD1	LEU 3	A 168	33.079	98.664	59.335	1.00 42.28	A	C
	ATOM	338	CD2			31.866		58.209	1.00 44.54	A	C
35	ATOM ATOM	339 340	C		A 168 A 168	34.702 33.974		54.851 53.884	1.00 49.49 1.00 49.80	A A	C
55	ATOM	341	N		A 169	35.806		54.756	1.00 51.68	A	N
	ATOM	342	CA		A 169	36.185		53.490	1.00 53.42	A	С
	ATOM	343	CB		A 169	37.063		53.749	1.00 53.84	A	С
40	MOTA MOTA	344 345	CD		A 169	38.381		54.394	1.00 54.96 1.00 55.82	A	C
40	ATOM	345	OE1		A 169 A 169	39.178 38.781	100.665	54.697 55.619	1.00 55.82	A A	C
	ATOM	347	OE2		169	40.193		54.006	1.00 57.62	A	ŏ
	ATOM	348	C		A 169	36.886	97.589	52.523	1.00 53.75	A	C
45	MOTA	349	0		A 169	37.892		51.922	1.00 54.54	A	0
45	ATOM ATOM	350 351	N CA		A 170 A 170	36.352 36.923	96.382 95.398	52.375 51.464	1.00 54.68 1.00 55.27	A A	N
	ATOM	352	CB		170	38.040		52.151	1.00 56.80	Â	č
	ATOM	353	CG	LYS 2	A 170	37.588	93.641	53.249	1.00 59.09	A	C
	ATOM	354	CD		A 170	37.396		52.725	1.00 59.63	A	C
50	ATOM ATOM	355 356	CE		A 170 A 170	37.133 37.117	91.239 89.809	53.873 53.437	1.00 60.14 1.00 59.19	A A	C
	ATOM	357	C		A 170	35.815	94.469	50.997	1.00 55.75	A	C
	ATOM	358	ō		A 170	35.765		49.830	1.00 56.27	A	ō
	ATOM	359	N		A 171	34.921	94.116	51.915	1.00 55.93	A	1/1
55	MOTA	360	CA		A 171	33.792		51.590	1.00 56.64	A	c
	MOTA	361 362	CB		A 171 A 171	33.064 32.872		52.866 50.719	1.00 56.68 1.00 56.98	A A	C
	ATOM	363	ō		A 171	31.899	93.599	50.139	1.00 55.93	A	ō
	MOTA	364	N		172	33.207	95.369	50.642	1.00 56.93	A	N
60	MOTA	365	CA		A 172	32.429		49.856	1.00 58.46	A	C
	MOTA	366	C		A 172	32.681	97.681	50.397	1.00 59.30	A	c
	ATOM	367 368	N		A 173	33.629 31.840		51.156 50.003	1.00 60.21 1.00 59.95	A A	N 0
	ATOM	369	CA	VAL 3	A 173	31.970	99.998	50.459	1.00 60.15	Ä	С
65	ATOM	370	CB	VAL 2	A 173	31.642	100.992	49.328	1.00 61.54	A	C
	MOTA	371	CG1		A 173	31.817		49.825	1.00 62.43	A	C
	ATOM ATOM	372 373	CG2 C		A 173 A 173	32.538 30.955		48.118 51.574	1.00 61.17 1.00 59.92	A A	c
	ATOM	374	0		A 173	29.860		51.369	1.00 59.92	A	0
70	ATOM	375	N	GLU 2	A 174	31.327	99.652	52.756	1.00 58.81	A	N
	ATOM	376	CA		A 174	30.452		53.921	1.00 55.71	A	С
	MOTA	377	CB	GLU :	A 174	31.091	98.900	55.067	1.00 56.69	A	С

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	ATOM	378	CG	GLU	A 174	31.360 9	7.440	54.731	1.00 57.20	A	C
	ATOM	379	CD	GLU .		30.135 9	6.717	54.197	1.00 57.78	A	C
	ATOM	380	OE1		A 174		7.156	53.166	1.00 56.65	A	0
-	ATOM	381	OE2		A 174		5.705	54.808	1.00 57.97	Α	0
5	ATOM	382	C		A 174		1.040	54.428	1.00 54.20	A	C
	MOTA	383 384	0	GLU	A 174 A 175		1.302	55.634 53.506	1.00 53.74 1.00 51.35	A A	N
	ATOM ATOM	384	N CA		A 175		1.913 3.199	53.896	1.00 47.97	A	C
	ATOM	386	CB		A 175		4.184	52.726	1.00 50.39	A	c
10	ATOM	387	CG	HIS			4.788	52.460	1.00 54.57	A	č
10	ATOM	388		HIS			5.144	51.303	1.00 55.04	λ	č
	ATOM	389		HIS			5.127	53.472	1.00 55.47	A	N
	ATOM	390		HIS			5.664	52.949	1.00 55.64	A	C
	ATOM	391	NE2	HIS	A 175	32.216 10	5.687	51.635	1.00 55.68	A	N
15	MOTA	392	C		A 175		2.794	54.253	1.00 44.77	A	C
	ATOM	393	0		A 175		3.562	54.817	1.00 43.37	A	0
	MOTA	394	34		A 176		01.550	53.902 54.178	1.00 41.61 1.00 39.54	A	N
	ATOM ATOM	395 396	CB		A 176 A 176		9.524	53.604	1.00 39.34	A A	c
20	ATOM	397	CG		A 176		8.672	54.086	1.00 42.14	A	č
20	ATOM	398	co		A 176		9.184	53.606	1.00 44.16	A	č
	ATOM	399	OE1		A 176		8.673	54.002	1.00 45.91	A	ŏ
	ATOM	400	NE2		A 176		0.193	52.745	1.00 43.65	A	N
	ATOM	401	C		A 176		0.891	55.696	1.00 37.68	A	C
25	ATOM	402	0		A 176		1.142	56.205	1.00 36.70	A	0
	ATOM	403	N		A 177		0.559	56.408	1.00 34.73	A	30
	ATOM	404	CA		A 177		0.495	57.862	1.00 33.53	A	C
	ATOM	405	CB		A 177		0.230	58.427	1.00 32.47	A	c
20	ATOM	406	CG		A 177	28.307 10	00.187	59.957	1.00 32.80	A	C
30	ATOM ATOM	407 408	CD1		A 177 A 177		98.844	60.439 60.431	1.00 33.65 1.00 31.75	A A	c
	ATOM	408	CDZ		A 177		1.842	58.380	1.00 33.15	A	č
	ATOM	410	ŏ		A 177		1.920	59.168	1.00 30.88	A	ŏ
	ATOM	411	N		A 178		2.898	57.916	1.00 31.91	A	N
35	ATOM	412	CA		A 178		04.261	58.317	1.00 31.40	A	C
	ATOM	413	CB	ARG	A 178	27.661 10	5.238	57.618	1.00 33.75	A	C
	ATOM	414	CG		A 178		6.625	58.226	1.00 36.73	A	C
	ATOM	415	CD		A 178		7.531	57.562	1.00 43.53	A	C
	ATOM	416	NE		A 178		8.809	58.262	1.00 46.96	A	N
40	ATOM	417	CZ		A 178		9.770	57.909	1.00 48.25	A A	C
	ATOM	418 419	NH1 NH2		A 178 A 178		09.604 L0.895	56.857 58.613	1.00 48.99 1.00 47.98	A	N
	ATOM	420	C		A 178		14.669	58.065	1.00 29.09	A	c
	ATOM	421	ŏ		A 178		5.327	58.902	1.00 28.32	A	ō
45	ATOM	422	N		A 179		04.289	56.924	1.00 28.97	A	N
	ATOM	423	CA	ARG	A 179	23.301 10	4.633	56.624	1.00 27.69	A	C
	MOTA	424	CB		A 179		14.220	55.194	1.00 29.53	A	C
	MOTA	425	CG		A 179	23.091 10		54.131	1.00 33.34	A	С
	MOTA	426	CD		A 179	22.514 10		52.800	1.00 34.69	A	C
50	MOTA	427	NE		A 179	21.091 10		52.896	1.00 38.29	A A	N
	MOTA	428 429	CZ NH1		A 179 A 179		05.367	52.916 52.842	1.00 39.89 1.00 41.81	A	N
	ATOM	430	NH2	ARG	A 179	18.840 10	14 966	53.011	1.00 39.44	A	N
	MOTA	431	C		A 179		3.900	57.589	1.00 25.80	Ä	è
55	ATOM	432	ŏ		A 179	21.421 10		58.121	1.00 24.65	A	ō
	ATOM	433	N		A 180	22.689 10	02.628	57.795	1.00 24.97	A	N
	ATOM	434	CA		A 180	21.924 10	01.746	58.655	1.00 24.64	A	C
	ATOM	435	CB		A 180	22.475 10	00.329	58.512	1.00 25.95	A	C
	ATOM	436	CG		A 180		99.239	58.900	1.00 30.77	A	C
60	ATOM	437	CD		A 180		99.256	58.073	1.00 32.75	A	C
	ATOM	438	OE1		A 180		99.283	56.830	1.00 33.51	A A	0
	ATOM	439 440	OE2		A 180 A 180		99.233	58.669 60.110	1.00 36.77 1.00 24.56	A	C
	ATOM	441	0		A 180		02.116	60.831	1.00 24.50	A	Ö
65	ATOM	442	N		A 181		02.715	60.541	1.00 23.97	A	N
00	ATOM	443	CA		A 181	23.235 10		61.905	1.00 25.68	A	C
	ATOM	444	CB		A 181	24.709 10		62.244	1.00 24.65	A	C
	ATOM	445	CG1	VAL	A 181	24.806 10	04.314	63.499	1.00 21.02	A	C
	ATOM	446	CG2		A 181	25.440 10		62.440	1.00 23.99	A	C
70	MOTA	447	С		A 181	22.403 10		62.100	1.00 27.42	A	C
	ATOM	448	0		A 181	21.771 10		63.144	1.00 28.13	A	O
	MOTA	449	N	GLU	A 182	22.406 10	05.30/	61.079	1.00 28.83	A	24

						-51-				
	ATOM	450	CA		A 182	21.667 106.56		1.00 31.06	A	C
	ATOM	451	CB		A 182	21.938 107.33		1.00 34.99	A	C
	ATOM	452	CD		A 182	21.403 108.75		1.00 41.26 1.00 45.14	A A	C
5	ATOM	453 454			A 182 A 182	21.846 109.42 21.502 110.6		1.00 45.14	A	ŏ
-	ATOM	455			A 182	22.548 108.75		1.00 46.92	A	ő
	MOTA	456	c	GLU	A 182	20.182 106.23	9 61.235	1.00 29.45	A	C
	MOTA	457	0		A 182	19.488 106.75		1.00 26.72	A	0
	MOTA	458	N		A 183	19.717 105.30		1.00 28.76	A	И
10	ATOM ATOM	459 460	CB		A 183 A 183	18.323 104.85 18.055 103.85		1.00 28.45 1.00 28.73	A A	C
	ATOM	461			A 183	16.618 103.4		1.00 28.72	A	č
	ATOM	462			A 183	18.344 104.5		1.00 27.67	A	C
	ATOM	463			A 183	18.250 103.60		1.00 26.58	A	C
15	ATOM	464	С		A 183	17.886 104.2		1.00 29.83	A	C
	ATOM	465	0		A 183	16.870 104.60 18.668 103.20		1.00 27.93 1.00 29.56	A	O N
	MOTA MOTA	466 467	N CA		A 184 A 184	18.349 102.5		1.00 30.04	A	C
	ATOM	468	CB		A 184	19.315 101.3		1.00 30.32	A	č
20	ATOM	469	CG		A 184	18.801 100.2		1.00 34.52	A	C
	MOTA	470	CD		A 184	17.721 99.4		1.00 32.90	A	C
	MOTA	471	OE1		A 184	16.988 98.69 17.628 99.4		1.00 36.44	A A	O N
	MOTA	472 473	NE2 C		A 184 A 184	17.628 99.4° 18.335 103.3		1.00 32.19	A	C
25	ATOM	474	ŏ		A 184	17.593 102.9		1.00 29.21	A	ŏ
	MOTA	475	N		A 185	19.139 104.3	75 64.752	1.00 32.70	A	N
	MOTA	476	CA		A 185	19.219 105.1	79 65.968	1.00 33.38	A	C
	MOTA	477	CB		A 185	20.512 105.9		1.00 34.25 1.00 35.32	A A	C
30	MOTA	478 479	OG C		A 185 A 185	20.460 107.0 18.051 106.1		1.00 35.32	A	c
30	ATOM	480	Ö		A 185	17.989 106.7		1.00 34.82	A	ŏ
	MOTA	481	N		A 186	17.131 106.2	12 65.237	1.00 35.78	A	N
	MOTA	482	CA		A 186	15.974 107.0	98 65.366	1.00 36.17	A	C
~-	MOTA	483	CB		A 186	15.875 108.0		1.00 38.62	A	C
35	ATOM ATOM	484 485	CG		A 186 A 186	17.044 108.9 17.816 109.5		1.00 42.07 1.00 42.75	A A	c
	ATOM	486			A 186	17.538 109.2		1.00 42.17	A	N
	ATOM	487			A 186	18.566 110.1		1.00 42.82	A	C
	ATOM	488			A 186	18.755 110.2		1.00 43.03	A	N
40		489	C		A 186	14.673 106.3		1.00 35.02 1.00 36.65	A A	C
	ATOM ATOM	490 491	O N		A 186 A 187	13.580 106.8 14.796 105.0		1.00 36.65	A	N
	ATOM	492	CA		A 187	13.631 104.1		1.00 29.84	A	С
	ATOM	493	CB		A 187	13.791 102.8	28 65.253	1.00 28.15	A	C
45	ATOM	494	CG		A 187	13.577 102.7		1.00 28.01	A	C
	ATOM	495			A 187	14.398 103.8		1.00 31.70 1.00 25.23	A	C
	ATOM ATOM	496 497	CD2		A 187 A 187	13.973 101.4 13.480 103.8		1.00 28.25	A	c
	ATOM	498	õ		A 187	14.397 103.3		1.00 28.90	Ä	ŏ
50	MOTA	499	N		A 188	12.333 104.2	54 68.038	1.00 25.67	A	N
	MOTA	500	CA		A 188	12.074 104.0	24 69.451	1.00 23.28	, A	C
	MOTA	501	CB		A 188	11.981 105.3		1.00 22.40	A	C
	MOTA	502 503	C		A 188 A 188	10.782 103.2 9.695 103.7		1.00 21.56 1.00 21.09	A A	0
55	MOTA	504	N		A 189	10.906 101.9		1.00 21.04	A	N
	ATOM	505	CA		A 189	9.736 101.0		1.00 22.71	A	C
	ATOM	506	CB		A 189	9.299 100.4		1.00 22.11	A	C
	MOTA	507	CG		A 189	7.961 99.7		1.00 23.56	A	C
60	ATOM ATOM	508 509			A 189 A 189	7.621 98.4 6.775 100.4		1.00 23.56	A A	N
JU.	ATOM	510			A 189	5.765 99.6			A	C
	ATOM	511		HIS	A 189	6.251 98.4	14 68.941	1.00 25.80	A	N
	ATOM	512	C	HIS	A 189	10.122 99.9	99 71.045		A	C
	MOTA	513	0	HIS	A 189	11.254 99.5			A A	O
65	ATOM	514 515	N CD	PRO	A 190 A 190	9.185 99.6 7.823 100.1			A A	C
	ATOM	516	CA		A 190	9.458 98.5	84 72.915	1.00 22.42	A	č
	MOTA	517	CB	PRO	A 190	8.238 98.6	59 73.837	1.00 22.67	A	C
	MOTA	518	CG		A 190	7.149 99.1		1.00 23.94	A	c
70	MOTA	519	C		A 190	9.688 97.1			A	C
	MOTA	520 521	O		A 190 A 191	10.091 96.2 9.445 97.0			A	N
	MION	221	14	27274	** TAT	9.443 97.0	70 17.043	2.00 21.27		

							-52-				
	ATOM	522	CA	ASN A	191	9.657	95.711	70.422	1.00 19.49	A	С
	ATOM	523	CB	ASN A		8.361	95.170	69.831	1.00 19.45	A	C
	MOTA	524	CG	ASN A		7.320	94.880	70.884	1.00 19.61	A	C
	MOTA	525		ASN A		7.495	93.995	71.715	1.00 22.06	A	0
5	ATOM	526		ASN A		6.227	95.628	70.855	1.00 20.03	A	C M
	MOTA	527	C	ASN A		10.732 10.813	95.753 94.857	69.345 68.497	1.00 19.88 1.00 19.36	A A	0
	MOTA	528	O N	ASN A		11.542	96.807	69.380	1.00 19.36	A	N
	ATOM	529 530	CA	ILE A		12,652	96.973	68.454	1.00 18.73	A	C
10	ATOM	531	CB	ILE A		12.412	98.160	67.491	1.00 18.58	A	č
10	ATOM	532		ILE A		13.676	98.453	66.697	1.00 15.53	A	Ċ
	ATOM	533	CG1	ILE A	192	11,252	97.824	66.543	1.00 20.81	A	C
	ATOM	534		ILE A	192	10.965	98.892	65.507	1.00 22.29	A	C
	ATOM	535	С	ILE A		13.904	97.224	69.300	1.00 19.43	A	C
15	ATOM	536	0	ILE A		13.909	98.111	70.157	1.00 21.71	A	0
	ATOM	537	N	LEU A		14.957	96.441	69.075 69.860	1.00 18.98	A A	N
	ATOM	538	CA	LEU A	193	16.188 17.214	96.588 95.514	69.860	1.00 20.69	A	c
	ATOM	539 540	CG	LEU A		18.234	95.514	70.558	1.00 19.99	A	č
20	ATOM	541		LEU A		17.560	94.248	71.601	1.00 18.84	Ä	č
20	ATOM	542		LEU A		19.431	94.424	69.942	1.00 20.29	A	c
	ATOM	543	c	LEU A		16.799	97.985	69.693	1.00 19.95	A	C
	ATOM	544	o	LEU A	193	17.020	98.455	68.578	1.00 21.40	A	0
	ATOM	545	N	ARG A		17.060	98.647	70.811	1.00 19.34	A	M
25	ATOM	546	CA	ARG A		17.628	99.988	70.805	1.00 18.88	A	c
	ATOM	547	CB	ARG A		17.376		72.154	1.00 23.30	A	c
	ATOM	548	CG	ARG A			101.460	72.259	1.00 29.13	A A	C
	ATOM	549	CD	ARG A		15.089	102.728 103.659	71.425	1.00 36.10	A	N
30	ATOM ATOM	550 551	CZ	ARG A		14.999		72.922	1.00 41.78	A	Ç
30	ATOM	552				15.925		73.860	1.00 45.72	A	N
	ATOM	553		ARG A		13.983		73.147	1.00 45.18	A	N
	ATOM	554	C	ARG A			100.073	70.513	1.00 18.39	A	С
	ATOM	555	0	ARG A	194	19.919	99.292	71.031	1.00 15.95	A	0
35	MOTA	556	N	LEU A		19.493		69.673	1.00 18.46	A	N
	MOTA	557	CA	LEU A	. 195	20.887		69.355	1.00 22.13	A	C
	ATOM	558	CB	LEU A	. 195		101.650	67.869	1.00 23.02	A	C
	ATOM	559	CG	LEU A	195		101.369	67.180 65.948	1.00 25.45	A A	C
40	ATOM	560 561	CDI		195		102.259 101.636	68.111	1.00 25.90	A	č
40	ATOM ATOM	562	CD2	LEU A	195		102.573	70.196	1.00 22.63	A	č
	ATOM	563	õ	LEU A	195		103.633	69.862	1.00 24.54	A	ō
	ATOM	564	N	TYR A	196		102.456	71.294	1.00 22.66	A	N
	ATOM	565	CA	TYR A	196	22.095		72.168	1.00 23.33	A	С
45	ATOM	566	CB	TYR A		22.619		73.534	1.00 22.65	A	C
	ATOM	567	CG	TYR A		21.702		74.310	1.00 21.37	A	C
	ATOM	568	CD1			22.190	101.040	74.879 75.677	1.00 22.83	A A	c
	MOTA	569 570		TYR A		21.387 20.379	102.565	74.551	1.00 22.12	A	č
50	ATOM	571	CE2			19.561	101.765	75.348	1.00 23.98	Ä	č
50	ATOM	572	CZ	TYR A		20.075		75.911	1.00 25.61	A	c
	ATOM	573	OH	TYR A		19.277	99.825	76.725	1.00 27.32	A	0
	ATOM	574	C	TYR A		23.088	104.603	71.574	1.00 23.97	A	C
	MOTA	575	0	TYR A		23.028		71.867	1.00 24.83	A	0
55	ATOM	576	N	GLY F		24.008		70.750	1.00 25.27	A	M
	ATOM	577	CA	GLY 2		24.985		70.141 69.457	1.00 23.65 1.00 24.59	A A	C
	ATOM	578 579	C	GLY I		25.990	104.230	69.437	1.00 24.07	A	ŏ
	ATOM ATOM	580	N	TYR I		27.147		69.070	1.00 26.73	A	N
60	ATOM	581	CA	TYR /			104.307	68.413	1.00 29.46	A	c
00	ATOM	582	CB	TYR A			103.881	66.994	1.00 33.22	A	Ċ
	ATOM	583	CG	TYR /		27.914	104.997	65.981	1.00 38.83	A	C
	ATOM	584	CD1	TYR 2	198	29.029	105.197	65.165	1.00 40.36	A	C
	ATOM	585	CE1			29.066		64.237	1.00 44.11	A	c
65	MOTA	586	CD2			26.830		65.846	1.00 41.61	A	C
	ATOM	587	CE2			26.856	106.912	64.917	1.00 44.45	A	c
	MOTA	588 589	OH	TYR I		27.978 28.016		64.118 63.195	1.00 45.02 1.00 48.52	A A	0
	ATOM	589 590	C	TYR A		28.016		68.366	1.00 48.52	A	č
70	ATOM	591	0	TYR I		29.462		68.477	1.00 28.17	A	õ
,0	ATOM	592	N		199		104.729	68.218	1.00 30.25	A	N
	ATOM	593	CA	PHE			105.533	68.134	1.00 31.17	A	C

70 ATOM

ATOM 664 CG LEU A 207

A TYOM

663 CB LEU A 207

665

CD1 LEU A 207

27.183 99.001

27.574 99.160

26.675 98.309

67.288

65.814

1.00 21.53

1.00 21.15

64.950 1.00 23.10

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	MOTA	666			A 207	27.462	100.624	65.412	1.00 23.96	A	C
	MOTA MOTA	667 668	C		A 207 A 207	27.495 27.760	99.542	69.712 70.204	1.00 20.27	A A	C
	ATOM	669	N		A 207	26.825	98.443 100.480	70.204	1.00 22.20 1.00 18.68	A	N
5	ATOM	670	CA		A 208	26.350	100.256	71.736	1.00 18.33	Ä	C
	MOTA	671	СВ		A 208	26.514	101.518	72.599	1.00 17.78	A	C
	MOTA MOTA	672 673	CG2 CG1		A 208 A 208	26.331 27.896	101.161	74.075 72.365	1.00 18.29 1.00 21.18	A	C
	ATOM	674			A 208	28.100	103.468	73.086	1.00 21.18	A	c
10	MOTA	675	c	ILE	A 208	24.864	99.895	71.650	1.00 19.02	A	C
	ATOM	676	0		A 208	24.025	100.749	71.332	1.00 20.96	A	0
	MOTA MOTA	677 678	N CA		A 209 A 209	24.554 23.200	98.639 98.100	71.963 71.868	1.00 18.23	A A	C N
	ATOM	679	CB		A 209	23.216	96.893	70.941	1.00 17.32	A	č
15	MOTA	680	CG	LEU	A 209	23.871	97.022	69.564	1.00 19.38	A	C
	MOTA	681	CD1		A 209	24.381	95.647	69.117	1.00 20.09	A	C
	MOTA	682 683	CD2		A 209 A 209	22.877 22.519	97.587 97.668	68.571 73.160	1.00 19.54 1.00 19.32	A A	C
	ATOM	684	ŏ		A 209	23.169	97.322	74.149	1.00 19.32	A	Ö
20	MOTA	685	N	GLU	A 210	21.190	97.682	73.124	1.00 17.29	A	N
	ATOM	686	CA		A 210	20.373	97.235	74.240	1.00 17.08	A	C
	ATOM ATOM	687 688	CB		A 210 A 210	18.892 17.915	97.490 97.005	73.922 74.971	1.00 17.25 1.00 14.08	A A	C
	ATOM	689	CD		A 210	16.466	97.056	74.493	1.00 16.64	A	c
25	ATOM	690	OE1	GLU	A 210	15.579	96.672	75.275	1.00 16.48	A	ŏ
	ATOM	691	OE2		A 210	16.210	97.470	73.338	1.00 18.70	A	0
	ATOM ATOM	692 693	C		A 210 A 210	20.625 20.722	95.724 95.018	74.369 73.367	1.00 17.70 1.00 16.33	A A	C
	ATOM	694	N		A 210	20.722	95.018	75.596	1.00 18.33	A	N
30	ATOM	695	CA		A 211	20.992	93.811	75.817	1.00 18.22	A	C
	ATOM	696	CB		A 211	21.889	93.644	77.045	1.00 21.03	A	C
	ATOM ATOM	697 698	CD1		A 211 A 211	22.150 22.898	92.216 91.347	77.474 76.681	1.00 21.77 1.00 22.50	A A	C
	ATOM	699	CE1		A 211	23.160	90.036	77.103	1.00 22.50	A	c
35	ATOM	700	CD2		A 211	21.671	91.743	78.696	1.00 22.56	A	č
	ATOM	701	CE2		A 211	21.928	90.443	79.124	1.00 21.84	A	C
	ATOM	702	CZ		A 211	22.666	89.598	78.328	1.00 22.93	A	C
	ATOM ATOM	703 704	OH		A 211 A 211	22.902 19.704	88.314 93.011	78.757 75.996	1.00 24.56	A A	0
40	ATOM	705	ŏ		A 211	18.791	93.444	76.694	1.00 16.95	A	ŏ
	ATOM	706	N		A 212	19.642	91.845	75.353	1.00 18.77	A	N
	ATOM ATOM	707 708	CB		A 212 A 212	18.477 18.090	90.952 90.485	75.439 74.040	1.00 18.90 1.00 16.75	A A	C
	ATOM	709	C.		A 212	18.873	89.755	76.325	1.00 19.85	A	c
45	ATOM	710	0	ALA	A 212	19.551	88.837	75.872	1.00 20.40	A	0
	ATOM	711	N		A 213	18.444	89.757	77.602	1.00 21.83	A	N
	ATOM ATOM	712 713	CD		A 213 A 213	17.600 18.727	90.806 88.726	78.190 78.609	1.00 22.17 1.00 22.10	A A	C
	ATOM	714	CB		A 213	18.026	89.258	79.865	1.00 23.45	Ä	c
50	ATOM	715	CG	PRO	A 213	17.976	90.713	79.651	1.00 24.12	A	C
	ATOM	716	С		A 213	18.318	87.295	78.320	1.00 22.31	A	С
	ATOM ATOM	717 718	O N	PRO	A 213 A 214	19.019 17.184	86.360 87.111	78.703 77.656	1.00 22.54 1.00 22.59	A A	O N
	ATOM	719	CA	LEU		16.715	85.765	77.375	1.00 20.79	A	č
55	ATOM	720	CB	LEU	A 214	15.181	85.716	77.499	1.00 21.06	A	C
	MOTA	721 722	CG		A 214 A 214	14.680 15.249	85.611	78.950	1.00 22.27	A	c
	ATOM ATOM	723	CD1	LEU		13.160	86.752 85.633	79.769 79.001	1.00 25.21	A A	c
	ATOM	724	C		A 214	17.189	85.117	76.075	1.00 20.41	A	č
60	ATOM	725	0	PEA		16.846	83.975	75.805	1.00 21.99	A	0
	ATOM	726	N		A 215	17.986	85.823	75.276	1.00 20.34	A	N
	ATOM	727 728	CA C		A 215 A 215	18.503 17.611	85.227 85.190	74.047 72.813	1.00 22.43 1.00 21.59	A A	C
	MOTA	729	0	GLY	A 215	16.679	85.976	72.696	1.00 23.24	A	õ
65	ATOM	730	N	THR	A 216	17.892	84.273	71.889	1.00 22.02	A	N
	ATOM ATOM	731 732	CA		A 216 A 216	17.112	84.172	70.652	1.00 23.73	A	C
	ATOM	732	OG1		A 216	17.960 18.233	83.626 82.238	69.487 69.706	1.00 24.78 1.00 25.51	A A	C
	ATOM	734	CG2		A 216	19.270	84.397	69.369	1.00 25.01	A	c
70	ATOM	735	C	THR	A 216	15.851	83.314	70.720	1.00 23.31	A	C
	ATOM	736	O		A 216 A 217	15.750	82.382	71.513	1.00 21.80	A	0
	MOTA	737	N	ANT	n 21/	14.886	83.645	69.867	1.00 25.09	A	N

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	MOTA	738	CA		A 217	13.626	82.904	69.797	1.00 25.79	A	C
	ATOM	739	CB		A 217	12.604	83.633	68.902	1.00 23.02	A	C
	ATOM	740			A 217	11.368	82.773	68.703	1.00 24.17	A	C
5	ATOM	741 742	CG2		A 217 A 217	12.234 13.921	84.961 81.530	69.533	1.00 22.94	A	C
,	ATOM	743	ŏ		A 217	13.278	80.534	69.196 69.525	1.00 26.14 1.00 25.55	A A	C
	ATOM	744	N		A 218	14.909	81.501	68.314	1.00 26.45	A	N
	ATOM	745	CA	TYR	A 218	15.327	80.283	67.655	1.00 30.04	A	C
	MOTA	746	CB	TYR	A 218	16.464	80.624	66.690	1.00 34.58	A	С
10	ATOM	747	CG		A 218	17.201	79.443	66.113	1.00 40.28	A	C
	ATOM	748 749	CE1		A 218 A 218	18.240 18.945	78.834 77.765	66.818 66.277	1.00 43.24 1.00 44.89	A	C
	ATOM	750	CD2		A 218	16.882	78.949	64.854	1.00 42.24	A	C
	ATOM	751	CE2		A 218	17.579	77.879	64.304	1.00 44.73	A	č
15	MOTA	752	cz	TYR	A 218	18.608	77.292	65.019	1.00 46.29	A	č
	MOTA	753	OH		A 218	19.304	76.235	64.475	1.00 48.71	A	0
	ATOM ATOM	754 755	C	TYR	A 218	15.759	79.241	68.684	1.00 30.04	A	C
	ATOM	756	N		A 218 A 219	15.383 16.534	78.075 79.675	68.607 69.668	1.00 29.65 1.00 31.08	A A	O N
20	ATOM	757	CA		A 219	17.011	78.778	70.702	1.00 30.24	A	C
	ATOM	758	CB		A 219	18.047	79.502	71.555	1.00 34.57	A	č
	MOTA	759	CG		A 219	18.660	78.657	72.634	1.00 39.81	A	C
	ATOM	760	CD		A 219	19.723	79.443	73.374	1.00 45.90	A	C
25	MOTA	761 762	NE		A 219 A 219	20.255 21.250	78.683 79.097	74.501 75.276	1.00 51.60	A	N
23	ATOM	763			A 219	21.250	80.273	75.276	1.00 52.82 1.00 53.30	A A	C
	MOTA	764			A 219	21.658	78.338	76.289	1.00 53.23	A	N
	MOTA	765	С		A 219	15.855	78.267	71.556	1.00 29.44	A	c
	ATOM	766	0		A 219	15.829	77.101	71.941	1.00 28.48	A	0
30	ATOM	767	N		A 220	14.892	79.138	71.840	1.00 29.18	A	N
	ATOM ATOM	768 769	CA		A 220 A 220	13.721 12.873	78.765 80.011	72.627 72.924	1.00 29.90 1.00 30.93	A A	C
	ATOM	770	CG		A 220	11.570	79.737	73.653	1.00 35.19	A	č
	ATOM	771	CD		A 220	10.684	80.975	73.765	1.00 38.55	A	č
35	ATOM	772	OE1		A 220	10.619	81.754	72.789	1.00 41.41	A	0
	ATOM	773	OE2		A 220	10.036	81.165	74.816	1.00 38.75	A	0
	ATOM	774 775	C		A 220 A 220	12.890	77.730	71.852	1.00 29.28 1.00 29.27	A	C
	ATOM	776	N		A 220 A 221	12.319 12.846	76.813 77.882	72.434	1.00 29.27	A A	O N
40	ATOM	777	CA		A 221	12.096	76.981	69.661	1.00 29.41	A	Č
	ATOM	778	CB	LEU	A 221	12.087	77.547	68.234	1.00 29.75	A	C
	ATOM	779	CG	LEU	A 221	11.135	76.947	67.198	1.00 27.34	A	C
	ATOM	780 781			A 221 A 221	9.691 11.298	77.040 77.707	67.681	1.00 26.36	A	C
45	ATOM	782	CDA		A 221	12.691	75.570	65.902 69.655	1.00 28.29 1.00 31.02	A A	C
	ATOM	783	ŏ		A 221	11.958	74.579	69.659	1.00 30.54	A	ō
	ATOM	784	N	GLN	A 222	14.022	75.487	69.636	1.00 32.15	A	N
	MOTA	785	CA		A 222	14.718	74.204	69.644	1.00 33.38	A	C
50	ATOM ATOM	786 787	CB		A 222 A 222	16.224 16.624	74.405	69.478	1.00 36.12	A	C
50	ATOM	788	CD		A 222	18.126	75.120 75.279	68.206 68.092	1.00 40.81 1.00 44.96	A A	C
	ATOM	789	OE1		A 222	18.787	75.722	69.033	1.00 46.46	A	o
	ATOM	790	NE2		A 222	18.675	74.924	66.933	1.00 47.81	A	N
	ATOM	791	С		A 222	14.467	73.437	70.937	1.00 33.08	A	C
55	ATOM	792 793	N		A 222 A 223	14.435 14.288	72.212 74.160	70.933 72.038	1.00 33.65	A	0
	ATOM	794	CA		A 223	14.288	73.539	73.336	1.00 32.99 1.00 32.56	A A	C N
	ATOM	795	CB		A 223	14.314	74.541	74.464	1.00 35.07	A	č
	ATOM	796	CG		A 223	15.780	74.660	74.873	1.00 38.94	A	č
60	ATOM	797	CD		A 223	16.682	74.938	73.680	1.00 42.58	A	C
	MOTA	798 799	CE NZ		A 223	18.143	75.049	74.084	1.00 45.75	A	C
	ATOM	800	C NZ		A 223 A 223	19.012 12.629	75.377 72.992	72.910 73.480	1.00 47.32 1.00 31.92	A A	N
	ATOM	801	Ö		A 223	12.444	72.992	73.480	1.00 31.92	A A	0
65	ATOM	802	N	LEU	A 224	11.635	73.815	73.159	1.00 29.58	A	N
	ATOM	803	CA	PEA	A 224	10.235	73.413	73.272	1.00 27.04	A	C
	ATOM	804	CB		A 224	9.355	74.651	73.488	1.00 27.41	A	C
	ATOM	805 806	CG CD1		A 224 A 224	9.626 8.545	75.554 76.626	74.703 74.805	1.00 26.07 1.00 23.48	A A	C
70	ATOM	807	CD2	LEU	A 224	9.632	74.717	75.968	1.00 25.48	A A	C
	MOTA	808	C	LEU	A 224	9.698	72.613	72.080	1.00 26.87	Ä	c
	MOTA	809	0		A 224	8.653	71.977	72.187	1.00 27.46	A	ō

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	ATOM	810	N	CHD	A 225	10.410	-56- 72.650	70.954	1.00 26.55	А	N
	ATOM	811	CA		A 225	10.009	71.944	69.730	1.00 28.34	A	c
	ATOM	812	CB		A 225	9.473	70.549	70.062	1.00 30.23	A	c
	ATOM	813	OG		A 225	9.605	69.698	68.941	1.00 33.93	A	0
5	ATOM	814	C		A 225	8.964	72.732	68.920	1.00 26.55	A	C
	ATOM	815	0		A 225	9.046	72.810	67.697	1.00 26.63	A	0
	ATOM	816 817	N CA		A 226 A 226	7.977 6.958	73.296 74.129	69.607 68.976	1.00 25.84 1.00 25.88	A A	C
	ATOM	818	CB		A 226	6.012	73.304	68.087	1.00 28.21	A	c
10		819	CG		A 226	5.184	72.259	68.790	1.00 28.88	A	č
	ATOM	820	CD		A 226	4.409	71.443	67.770	1.00 34.11	A	C
	MOTA	821	CE		A 226	3.483	70.427	68.435	1.00 34.70	A	С
	ATOM	822	NZ		A 226	4.240	69.444	69.261	1.00 37.81	A	N
16	ATOM	823	C		A 226	6.191	74.851	70.073	1.00 25.27	A	C
15	ATOM	824 825	N		A 226 A 227	6.124 5.637	74.373 76.016	71.202 69.749	1.00 26.71 1.00 24.65	A A	N
	ATOM	826	CA		A 227	4.891	76.808	70.722	1.00 22.54	A	C
	ATOM	827	СВ		A 227	5.085	78.312	70.463	1.00 23.44	A	c
	MOTA	828	CG		A 227	6.527	78.753	70.359	1.00 20.95	A	C
20	MOTA	829			A 227	7.523	78.135	71.106	1.00 21.88	A	C
	MOTA	830			A 227	6.868	79.847	69.561	1.00 19.95	A	c
	MOTA	831 832			A 227 A 227	8.850 8.183	78.606 80.326	71.065 69.511	1.00 23.78 1.00 21.33	A A	C
	MOTA	833	CE2		A 227	9.176	79.706	70.265	1.00 21.33	A	č
25	ATOM	834	c		A 227	3.397	76.514	70.673	1.00 22.04	A	č
	ATOM	835	ō		A 227	2.882	76.035	69.660	1.00 21.17	A	ò
	ATOM	836	N		A 228	2.707	76.813	71.768	1.00 19.93	A	N
	ATOM	837	CA		A 228	1.269	76.617	71.842	1.00 21.17	A	C
30	ATOM	838	CB		A 228	0.840	76.388	73.294	1.00 22.28	A	c
30	ATOM	839 840	CG OD1		A 228 A 228	1.204 1.715	77.547 77.288	74.203 75.307	1.00 24.14	A A	0
	ATOM	841			A 228	0.968	78.718	73.829	1.00 24.66	Â	ŏ
	ATOM	842	c		A 228	0.607	77.876	71.259	1.00 21.29	A	C
	ATOM	843	0		A 228	1.287	78.878	70.977	1.00 20.58	A	0
35	ATOM	844	N		A 229	-0.707	77.829	71.086	1.00 19.93	A	N
	ATOM	845	CA		A 229	-1.441	78.947	70.498	1.00 20.43	A A	c
	ATOM ATOM	846 847	CB		A 229 A 229	-2.919 -3.177	78.586 77.435	70.333 69.383	1.00 22.25	A	c
	ATOM	848	CD		A 229	-4.657	77.151	69.227	1.00 23.72	Ä	č
40	ATOM	849	OE1		A 229	-5.276	76.655	70.185	1.00 27.47	A	0
	ATOM	850			A 229	-5.203	77.437	68.152	1.00 23.78	A	0
	ATOM	851	С		A 229	-1.330	80.270	71.237	1.00 20.15	A	C
	ATOM	852 853	O N		A 229 A 230	-1.247 -1.337	81.320 80.238	70.598 72.569	1.00 19.16 1.00 17.98	A A	O
45	ATOM	854	CA		A 230	-1.233	81.480	73.319	1.00 17.46	Ä	č
	ATOM	855	CB		A 230	-1.412	81.246	74.833	1.00 16.42	A	č
	ATOM	856	CG		A 230	-1.448	82.560	75.641	1.00 18.34	A	C
	ATOM	857	CD		A 230	-1.683	82.377	77.140	1.00 18.98	A	С
50	ATOM	858	OE1		A 230	-0.744	82.430	77.933	1.00 21.19	A	0
50	ATOM	859 860	NE2 C		A 230 A 230	-2.932 0.107	82.167 82.173	77.529 73.040	1.00 16.82 1.00 16.75	A A	C M
	ATOM	861	ò		A 230	0.136	83.359	72.679	1.00 17.29	Ä	ŏ
	ATOM	862	N		A 231	1.210	81.443	73.179	1.00 14.85	A	N
	ATOM	863	CA	ARG	A 231	2.519	82.045	72.939	1.00 16.59	A	C
55	ATOM	864	CB		A 231	3.657	81.051	73.227	1.00 18.36	A	С
	ATOM	865	CG		A 231	5.042	81.728	73.190	1.00 22.57	A	c
	ATOM	866 867	CD		A 231 A 231	6.185 6.191	80.747 79.991	73.258 74.503	1.00 27.11 1.00 33.40	A A	N
	ATOM	868	CZ		A 231	6.654	80.446	75.664	1.00 35.76	A	Č
60	ATOM	869			A 231	6.605	79.675	76.738	1.00 36.21	A	N
	ATOM	870	NH2		A 231	7.176	81.660	75.752	1.00 38.74	A	N
	ATOM	871	С		A 231	2.671	82.581	71.513	1.00 14.93	A	C
	ATOM	872	0		A 231	3.151	83.700	71.311	1.00 14.16	A A	0
65	ATOM	873 874	N CA		A 232 A 232	2.276 2.366	81.776 82.160	70.531 69.121	1.00 15.57 1.00 17.08	A A	N.
05	ATOM	875	CB		A 232	1.859	81.030	68.188	1.00 17.08	A. A	c
	ATOM	876			A 232	2.656	79.856	68.382	1.00 18.40	A	0
	ATOM	877	CG2	THR	A 232	1.953	81.451	66.718	1.00 15.83	A	С
	ATOM	878	C		A 232	1.553	83.420	68.821	1.00 17.13	A	C
70	ATOM	879	0		A 232	2.061	84.359	68.204	1.00 18.70	A	N
	ATOM ATOM	880 881	N CA		A 233 A 233	0.296 -0.590	83.433 84.568	69.258 69.025	1.00 16.14 1.00 16.30	A A	C
	ATOM	991	CA	ana	A 233	-0.590	ue.508	03.025	1.00 10.30	A	-

	ATOM	882	СВ	מ ד מ	A 233	-1.982	-57- 84.246	69.529	1.00 16.62	A	C
	ATOM	883	CB		A 233	-0.076	85.846	69.529	1.00 16.62	A	č
	ATOM	884	ŏ		A 233	-0.259	86.944	69.166	1.00 16.10	A	ŏ
	ATOM	885	N	THR .	A 234	0.552	85.699	70.849	1.00 17.52	A	N
5	ATOM	886	CA	THR .		1.092	86.845	71.552	1.00 16.78	A	C
	ATOM	887	CB		A 234	1.494	86.467	73.014	1.00 17.54	A	C
	ATOM	888		THR .		0.314	86.125	73.759	1.00 12.72	A	0
	ATOM ATOM	889		THR .		2.184	87.633 87.362	73.706 70.766	1.00 17.21 1.00 16.02	A	C
10	ATOM	890 891	C	THR .	A 234 A 234	2.471	88.564	70.766	1.00 16.02 1.00 18.24	A A	Ö
10	ATOM	892	N		A 235	3.116	86.459	70.239	1.00 15.74	A	N
	ATOM	893	CA		A 235	4.275	86.879	69.456	1.00 18.00	A	Ĉ
	ATOM	894	CB	TYR .	A 235	5.180	85.694	69.117	1.00 18.40	A	C
	MOTA	895	CG	TYR .		6.016	85.167	70.264	1.00 22.59	A	C
15	ATOM	896	CD1	TYR		6.142	85.880	71.459	1.00 19.60	A	C
	ATOM	897 898	CE1	TYR .		6.943	85.413	72.490	1.00 23.79	A	C
	ATOM ATOM	898	CE2		A 235	6.718 7.530	83.968 83.492	70.133 71.158	1.00 22.03 1.00 25.06	A A	c
	ATOM	900	CZ		A 235	7.639	84.217	72.331	1.00 24.79	A	č
20	ATOM	901	OH		A 235	8.449	83.748	73.332	1.00 27.52	A	ŏ
	ATOM	902	C		A 235	3.882	87.574	68.148	1.00 17.48	A	Ċ
	ATOM	903	0		A 235	4.498	88.570	67.760	1.00 18.14	A	0
	ATOM	904	N		A 236	2.869	87.050	67.463	1.00 15.10	A	N
25	ATOM	905	CA		A 236	2.443	87.655	66.207	1.00 15.95	A	C
25	ATOM	906 907	CB CG2		A 236 A 236	1.374	86.784 87.425	65.505 64.184	1.00 15.91 1.00 14.22	A A	C
	ATOM	908	CG1		A 236	1.950	85.393	65.225	1.00 13.58	A	č
	ATOM	909	CD1		A 236	3.140	85.396	64.289	1.00 15.33	A	č
	ATOM	910	c		A 236	1.905	89.070	66.425	1.00 16.93	A	C
30	ATOM	911	0		A 236	2.064	89.935	65.560	1.00 16.24	A	0
	ATOM	912	N		A 237	1.281	89.301	67.584	1.00 18.11	A	N
	ATOM	913	CA	THR .		0.727	90.613	67.937	1.00 19.28	A	C
	ATOM	914 915	CB OG1	THR .	A 237 A 237	-0.107 -1.306	90.545 89.787	69.255 69.035	1.00 22.99	A	C
35	ATOM	916	CG2	THR		-0.470	91.953	69.741	1.00 21.39	A	č
-	ATOM	917	C	THR		1.863	91.610	68.152	1.00 19.31	A	č
	ATOM	918	ō	THR		1.787	92.763	67.726	1.00 20.31	A	ō
	ATOM	919	N		A 238	2.912	91.164	68.836	1.00 18.54	A	N
	ATOM	920	CA		A 238	4.063	92.011	69.097	1.00 18.15	A	C
40	ATOM	921 922	CB		A 238 A 238	5.052 4.684	91.280	70.025	1.00 20.31 1.00 23.11	A A	C
	ATOM	922	CD		A 238	5.394	91.396 90.392	72.410	1.00 23.11	A	c
	ATOM	924	OE1		A 238	6.516	89.946	72.079	1.00 24.03	A	ŏ
	ATOM	925	OE2		A 238	4.825	90.057	73.473	1.00 28.40	A	0
45	ATOM	926	С		A 238	4.746	92.432	67.794	1.00 17.67	A	C
	ATOM	927	0		A 238	5.101	93.601	67.629	1.00 16.64	A	0
	ATOM	928	N		A 239 A 239	4.917 5.555	91.487	66.869 65.573	1.00 18.93 1.00 19.50	A	N
	ATOM	929 930	CB		A 239	5.822	91.769	64.813	1.00 19.50	A A	C
50	ATOM	931	CG		A 239	6.841	89.501	65.407	1.00 23.44	A	č
	ATOM	932			A 239	6.766	88.159	64.674	1.00 22.23	A	č
	ATOM	933		LEU .		8.236	90.107	65.314	1.00 21.26	A	C
	ATOM	934	C	LEU .		4.727	92.703	64.675	1.00 19.61	A	С
55	ATOM	935	0		A 239	5.279	93.583	64.024	1.00 17.80	A	0
23	ATOM	936 937	N CA	ALA .		3.412 2.548	92.502 93.351	64.631 63.802	1.00 18.94	A A	N
	ATOM	938	CB	ALA .		1.079	92.853	63.841	1.00 18.09	A	č
	ATOM	939	C	ALA .		2.633	94.787	64.288	1.00 18.99	A	č
	ATOM	940	0	ALA.	A 240	2.721	95.706	63.482	1.00 22.48	A	0
60	ATOM	941	N		A 241	2.610	94.992	65.603	1.00 21.18	A	N
	ATOM	942	CA	ASN .		2.736	96.347	66.135	1.00 21.65	A	C
	ATOM	943	CB		A 241	2.687	96.365	67.663	1.00 23.20	A	C
	ATOM	944 945	CG OD1		A 241 A 241	1.299 0.325	96.153 96.621	68.203 67.626	1.00 24.44	A A	C
65	ATOM	946	ND2		A 241	1.198	95.462	69.326	1.00 27.36	λ	N
33	ATOM	947	C	ASN .		4.069	96.935	65.685	1.00 22.55	A	č
	ATOM	948	0	ASN		4.111	98.035	65.129	1.00 24.99	A	ő
	ATOM	949	N	ALA .		5.159	96.200	65.909	1.00 21.61	A	N
70	ATOM	950	CA	ALA .		6.483	96.684	65.525	1.00 20.55	A	C
/0	ATOM	951 952	CB C	ALA	A 242 A 242	7.557 6.607	95.687 96.967	65.959 64.026	1.00 20.38	A A	C
	ATOM	952	0		A 242	7.207	96.967	63.627	1.00 21.10	A A	0
	111044	333	,		444	7.207	21.509	03.027	1.00 20.03	Δ.	

ATOM 955 Ch LBU A 243 6.111 96.281 61.742 1.00 23.33 A ATOM 957 CO LBU A 243 6.556 93.828 61.128 1.00 21.88 A ATOM 957 CO LBU A 243 6.556 93.828 61.128 1.00 21.88 A ATOM 957 CO LBU A 243 6.556 93.828 61.556 61.557 1.00 20.110 A C ATOM 958 CO LBU A 243 7.848 93.828 61.556 61.557 1.00 20.110 A C ATOM 960 CD LBU A 243 7.848 91.648 7.489 61.00 21.69 A ATOM 961 O LBU A 243 7.849 91.495 1.00 21.69 A ATOM 962 N SER A 244 4.191 97.741 62.201 1.00 25.47 A ATOM 963 CO SER A 244 4.191 97.741 62.201 1.00 25.47 A ATOM 964 CO SER A 244 4.191 97.741 62.201 1.00 25.47 A ATOM 965 CO SER A 244 4.191 97.741 62.201 1.00 25.47 A ATOM 968 CO SER A 244 4.191 97.741 62.201 1.00 25.54 A A ATOM 969 CO SER A 244 4.191 97.741 62.201 1.00 25.54 A A A A A A A A A									-58-					
AROM 956 CB LBU A 243 5.617 95.029 61.014 1.00 21.81 A A A A A A A A A								6.050					7	
ATOM 957 CO LBU A 243 5.556 93.828 61.128 1.00 21.88 A A A A A A A A A														
5 AROM 958 CD1 LEUU A 243 5.843 92.565 60.657 1.00 20.10 A AROM 959 CD2 LEUU A 243 5.843 92.565 60.305 1.00 18.75 A CARDON 960 C LEUU A 243 5.244 97.489 61.306 1.00 23.369 A AROM 960 C LEUU A 243 5.244 97.489 61.306 1.00 23.369 A AROM 961 O LEUU A 243 5.244 97.489 61.306 1.00 23.369 A AROM 962 A SER A 244 4.195 97.897 62.894 1.00 22.16 A AROM 963 A SER A 244 4.195 97.897 62.894 1.00 22.16 A AROM 963 A AROM 963 A AROM 964 CD SER A 244 1.197 99.856 62.312 1.00 23.33 3 A AROM 965 OG SER A 244 1.177 99.856 62.312 1.00 27.14 A AROM 965 OG SER A 244 1.177 99.856 62.312 1.00 27.14 A AROM 967 O SER A 244 1.177 99.856 62.312 1.00 33.33 A AROM 967 O SER A 244 1.177 99.856 62.312 1.00 33.33 A AROM 967 O SER A 244 1.777 100.253 63.117 1.00 27.39 A 1 AROM 967 O SER A 244 1.777 100.253 63.117 1.00 27.39 A 1 AROM 967 O SER A 244 1.777 100.253 63.117 1.00 27.39 A 1 AROM 969 A TYR A 245 5.558 101.444 63.455 1.00 26.56 A AROM 969 A TYR A 245 5.558 101.444 63.455 1.00 26.56 A AROM 970 CD TYR A 245 5.558 101.444 63.455 1.00 26.56 A AROM 971 CD TYR A 245 6.836 102.088 65.248 1.00 26.61 A AROM 972 CD TYR A 245 6.836 103.580 65.709 1.00 26.61 A AROM 975 CD TYR A 245 6.836 103.580 65.248 1.00 26.18 A AROM 975 CD TYR A 245 9.517 103.008 65.248 1.00 26.18 A AROM 975 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 975 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 976 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.72 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 CD TYR A 245 9.517 103.008 65.248 1.00 27.61 A AROM 978 C														
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ATOM 1007 CE LYS A 249 8.754 107.506 63.231 1.00 39.69 A 65 A			1006		LYS	A	249			61.870				C C
ARCM 1009 C T/S A 249 9.457 105.048 58.012 1.00 34.43 A A A A A A A A A										63.231				
ATOM 1010 O LYS A 249 10.640 105.364 57.861 1.00 32.18 A 0 ATOM 1011 N ARG A 250 8.738 104.430 57.078 1.00 35.69 A 1 ATOM 1012 CA ARG A 250 9.288 104.081 55.778 1.00 37.56 A 0 ATOM 1013 CB ARG A 250 9.268 104.081 55.778 1.00 37.56 A 0 ATOM 1013 CB ARG A 250 9.666 105.359 55.038 1.00 41.59 A 0 ATOM 1015 CD ARG A 250 8.561 106.132 54.453 1.00 41.59 A 0 ATOM 1015 CD ARG A 250 8.501 106.132 54.453 1.00 41.59 A 0 ATOM 1015 CD ARG A 250 8.501 106.132 54.453 1.00 41.10 45.10 A 0 ATOM 1015 CD ARG A 250 8.232 107.855 52.679 1.00 47.20 A 1 ATOM 1018 NRI BARG A 250 8.232 107.855 52.679 1.00 47.20 A 1 ATOM 1019 NRI BARG A 250 8.232 107.855 52.679 1.00 47.20 A 1 ATOM 1010 NRI BARG A 250 8.232 107.855 52.679 1.00 47.20 A 1 ATOM 1019 NRI BARG A 250 8.042 107.863 50.381 1.00 44.57 A 1 ATOM 1020 C ARG A 250 10.465 103.118 55.890 1.00 48.77 A 1 ATOM 1020 C ARG A 250 10.465 103.118 55.890 1.00 88.88 A ATOM 1021 O ARG A 250 11.451 103.225 55.162 1.00 38.88 A ATOM 1021 O ARG A 250 11.451 103.225 55.162 1.00 38.88 A ATOM 1022 N VAL A 251 11.384 101.171 57.031 1.00 43.361 A ATOM 1024 CB VAL A 251 11.384 101.171 57.031 1.00 43.361 A ATOM 1024 CB VAL A 251 11.884 101.171 58.501 1.00 43.361 A	55				LYS	A	249							
ATOM 1011 N ARG A 250 8.738 104.430 57.078 1.00 35.5.69 A 1 ATOM 1012 CA ARGA A 250 9.686 105.359 55.038 1.00 37.56 A C ATOM 1013 CB ARG A 250 9.686 105.359 55.038 1.00 37.76 A C ATOM 1014 CD ARGA A 250 9.686 105.359 52.038 1.00 37.76 A C ATOM 1014 CD ARGA A 250 8.801 106.132 54.453 1.00 41.59 A C ATOM 1016 NE ARGA A 250 8.801 106.132 54.453 1.00 41.59 A C ATOM 1016 NE ARGA A 250 8.232 107.855 52.679 1.00 47.20 A A ATOM 1017 CE ARGA A 250 8.232 107.855 52.679 1.00 47.20 A A ATOM 1019 NIT2 ARGA A 250 9.865 106.884 51.374 1.00 46.33 A A ATOM 1019 NIT2 ARGA A 250 9.865 106.884 51.374 1.00 46.33 A A ATOM 1020 C ARGA A 250 10.465 103.118 55.890 1.00 45.77 A T ATOM 1020 C ARGA A 250 10.465 103.118 55.890 1.00 45.77 A T ATOM 1020 C ARGA A 250 10.465 103.118 55.890 1.00 39.53 A C ATOM 1020 C ARGA A 250 11.451 103.255 55.1.63 1.00 10.0 88.86 A C ATOM 1020 C ARGA A 250 11.451 103.255 55.1.63 1.00 38.86 A C ATOM 1020 C ARGA A 250 11.451 103.255 55.1.63 1.00 33.81 A C ATOM 1020 C ARGA A 250 11.451 103.255 55.1.63 1.00 33.45 A C ATOM 1020 C ARGA A 250 11.451 103.255 55.1.63 1.00 33.45 A C ATOM 1020 C AVAL A 251 11.384 101.171 57.031 1.00 43.51 A C														
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ATOM 1014 CG ARG A 250 8.501 106.132 54.463 1.00 41.59 A G ATOM 1015 CD ARG A 250 8.894 107.524 53.945 1.00 45.10 45.10 A C ATOM 1015 CD ARG A 250 8.232 107.855 52.679 1.00 47.20 A A ATOM 1017 CZ ARG A 250 8.232 107.855 52.679 1.00 47.20 A A ATOM 1017 CZ ARG A 250 9.865 106.884 51.374 1.00 47.18 A G ATOM 1019 NRI ARG A 250 9.865 106.884 51.374 1.00 47.18 A G ATOM 1019 NRI ARG A 250 9.865 106.884 51.374 1.00 46.33 A A ATOM 1019 NRI ARG A 250 9.865 106.884 51.374 1.00 45.73 A ATOM 1020 NRI ARG A 250 10.00 1		ATOM			ARG	A	250	9.288	104.081	55.778	1.00	37.56		C C
ATOM 1015 CD ARG A 250 8.894 107.524 53.945 1.00 45.10 A 6 ATOM 1016 NE ARG A 250 8.232 107.855 52.679 1.00 47.20 A 1 6 ATOM 1017 CZ ARG A 250 8.723 107.536 51.478 1.00 47.18 A 6 6 ATOM 1018 NH1 ARG A 250 9.865 106.884 51.374 1.00 46.33 A 1 ATOM 1019 NH2 ARG A 250 9.865 106.884 51.374 1.00 46.33 A 1 ATOM 1020 C ARG A 250 10.465 103.181 55.890 1.00 35.77 A 1 ATOM 1021 C ARG A 250 10.465 103.181 55.890 1.00 38.88 A 6 ATOM 1021 C ARG A 250 11.451 103.225 55.162 1.00 38.88 A 6 ATOM 1022 N VAL A 251 11.384 101.171 57.031 1.00 43.36 A 1 ATOM 1024 CB VAL A 251 11.384 101.171 57.031 1.00 43.36 A 1 ATOM 1024 CB VAL A 251 11.884 101.171 58.500 1.00 43.36 A 6 ATOM 1024	60													
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ATOM 1020 C ARG A 250 10.465 103.118 55.890 1.00 39.53 A ATOM 1021 O ARG A 250 11.451 103.225 55.162 1.00 38.88 A ATOM 1022 N VAL A 251 10.348 102.169 56.813 1.00 41.36 A TOM 1023 CA VAL A 251 11.384 101.171 57.031 1.00 43.361 A ATOM 1024 CB VAL A 251 11.846 101.171 58.500 1.00 43.34 A A A A A A A A A	65	ATOM			ARG	Α	250	9.865	106.884	51.374	1.00	46.33	I	. N
AROM 1021 O ARG A 250 11.451 103.225 55.162 1.00 38.88 A A AROM 1022 N VAL A 251 10.348 102.169 56.813 1.00 41.36 A 170 AROM 1023 CA VAL A 251 11.384 101.171 57.031 1.00 43.61 A AROM 1024 CB VAL A 251 11.846 101.171 57.031 1.00 43.61 A AROM 1024 CB VAL A 251 11.846 101.171 58.500 1.00 43.34 A AROM 1024 CB VAL A 251 11.846 101.171 58.500 A AROM 1024 CB VAL A 251 11.846 101.171 58.500 A AROM 1024 CB VAL A 251 11.846 101.171 58.500 A AROM 1024 CB VAL A 251 11.846 101.171 58.500 A AROM 1024 CB VAL A 251 11.846 101.171 58.500 A AROM 1024								8.042	107.863					
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	70		1023	CA	VAL	A	251	11.384	101.171	57.031				v C
ATOM 1025 CG1 VAL A 251 12.834 100.031 58.745 1.00 42.55 A (
		MOTA	1025	CG1	VAL	Α	251	12.834	100.031	58.745	1.00	42.55	I	C C

							-59-				
	ATOM	1026		VAL :			102.512	58.834	1.00 41.90	A	C
	ATOM	1027	С		A 251	10.864	99.782	56.672	1.00 45.77	A	С
	ATOM	1028 1029	N O		A 251 A 252	9.773 11.013	99.393 98.979	57.087 55.608	1.00 45.19 1.00 48.92	A	0
5	ATOM	1029	CA		A 252	10.490	97.678	55.184	1.00 48.92	A A	C
-	ATOM	1031	CB		A 252	10.035	97.701	53.702	1.00 51.65	A	č
	ATOM	1032	CG2		A 252	9.532	96.322	53.292	1.00 52.57	A	č
	ATOM	1033	CG1		A 252	8.929	98.741	53.511	1.00 50.23	A	С
10	ATOM	1034	CD1		A 252	9.375		53.722	1.00 48.71	A	С
10	ATOM	1035 1036	C		A 252 A 252	11.630 12.743	96.682 96.924	55.358 54.895	1.00 53.81 1.00 53.23	A A	C
	ATOM	1037	N		A 253	11.359	95.564	56.019	1.00 57.15	A	N
	ATOM	1038	CA		A 253	12.415	94.593	56.281	1.00 60.73	Ä	č
	ATOM	1039	CB		A 253	12.150	93.878	57.606	1.00 61.57	A	C
15	ATOM	1040	CG		A 253	12.383	94.743	58.805	1.00 63.18	A	С
	ATOM	1041	CD2 ND1	HIS I		11.736	94.819	59.992	1.00 62.71	A	C
	ATOM	1042		HIS		13.419 13.400	95.651 96.248	58.873 60.051	1.00 63.35 1.00 63.74	A A	N
	ATOM	1044		HIS		12.389	95.762	60.749	1.00 63.74	Ä	N
20	ATOM	1045	C		A 253	12.749	93.565	55.217	1.00 62.30	A	c
	ATOM	1046	0		A 253	13.885	93.514	54.744	1.00 61.97	A	0
	ATOM	1047	N		A 254	11.774	92.742	54.849	1.00 64.77	A	N
	ATOM ATOM	1048	CA CB		A 254 A 254	12.004 12.719	91.700 92.304	53.855 52.639	1.00 66.63 1.00 67.76	A A	C
25	ATOM	1050	CG		A 254	11.948	93.473	52.639	1.00 69.83	A	C
	ATOM	1051	CD		A 254	12.846	94.466	51.288	1.00 71.13	A	č
	ATOM	1052	NE	ARG :	A 254	13.615	93.863	50.203	1.00 71.83	A	N
	ATOM	1053	CZ		A 254	14.438	94.543	49.410	1.00 72.27	A	C
30	ATOM ATOM	1054 1055		ARG		14.596	95.850	49.580	1.00 72.84	A	N
30	ATOM	1056	C NH2	ARG :	A 254	15.107 12.858	93.917	48.450 54.507	1.00 72.64	A A	N
	ATOM	1057	ŏ		254	13.356	89.699	53.830	1.00 67.13	A	ŏ
	ATOM	1058	N	ASP 2	A 255	13.002	90.694	55.832	1.00 67.58	A	N
	MOTA	1059	CA		A 255	13.789	89.744	56.630	1.00 66.56	A	C
35	ATOM	1060	CB	ASP 3		15.286	90.046	56.458	1.00 67.69	A	C
	ATOM ATOM	1061 1062	CG	ASP A		16.113 16.108	89.642 88.448	57.669 58.041	1.00 68.95 1.00 69.89	A A	C
	ATOM	1063		ASP 2		16.772	90.529	58.249	1.00 69.16	A	0
	ATOM	1064	C	ASP :		13.413	89.809	58.122	1.00 64.41	A	č
40	ATOM	1065	0	ASP 2		13.261	90.904	58.674	1.00 64.57	A	0
	ATOM	1066	N		256	13.265	88.644	58.763	1.00 60.26	A	N
	ATOM	1067 1068	CB		A 256 A 256	12.918 11.560	88.587 89.297	60.186 60.443	1.00 56.43 1.00 56.10	A A	C
	ATOM	1069	CG2	ILE 2		10.406	88.449	59.934	1.00 55.25	A	c
45	ATOM	1070	CG1			11.386	89.571	61.931	1.00 55.17	A	č
	MOTA	1071	CD1	ILE 2		10.193	90.444	62.235	1.00 56.51	A	C
	ATOM	1072	C	ILE :		12.877	87.163	60.782	1.00 53.68	A	C
	ATOM	1073 1074	O N	LYS	256	11.950 13.904	86.803 86.370	61.505 60.492	1.00 53.90 1.00 49.81	A A	N
50	ATOM	1075	CA	LYS		14.008	84.992	60.492	1.00 46.01	A	C
	ATOM	1076	CB	LYS		15.248	84.327	60.369	1.00 45.90	A	č
	ATOM	1077	CG	LYS 2		15.162	84.086	58.880	1.00 48.40	A	C
	ATOM	1078	CD	LYS 2		16.403	83.366	58.365	1.00 49.60	A	C
55	ATOM	1079 1080	CE NZ	LYS I		17.628 17.476	84.250 85.429	58.442	1.00 49.74 1.00 51.45	A	C
33	ATOM	1081	C	LYS		14.070	84.838	62.498	1.00 51.45	A A	И
	ATOM	1082	ŏ	LYS 2		14.379	85.783	63.218	1.00 42.43	A	ŏ
	ATOM	1083	N	PRO 2		13.822	84.410	63.074	1.00 38.37	A	N
	ATOM	1084	CD	PRO 2		13.620	83.540	61.908	1.00 37.81	A	C
60	ATOM	1085 1086	CA	PRO 2		13.838	83.621	64.315	1.00 36.58	A	С
	ATOM	1086	CB	PRO 2		13.569 12.869	82.193 82.383	63.834 62.514	1.00 35.41 1.00 35.75	A A	C
	ATOM	1088	C		1 258	15.216	83.756	64.962	1.00 35.75	A	c
	ATOM	1089	0	PRO 2	258	15.333	84.057	66.151	1.00 32.14	A	ŏ
65	MOTA	1090	N	GLU 2		16.249	83.523	64.155	1.00 35.08	A	N
	ATOM	1091	CA	GLU 2		17.626	83.652	64.601	1.00 36.22	A	C
	ATOM	1092 1093	CB	GLU 2	259	18.607 18.795	83.198 81.688	63.506	1.00 37.23	A	C
	ATOM	1094	co	GLU 2	259	17.713	81.688	63.340 62.496	1.00 40.19 1.00 42.23	A A	C
70	ATOM	1095	OE1	GLU 2	259	17.915	79.827	62.142	1.00 41.52	A	ŏ
	ATOM	1096		GLU 2	259	16.670	81.642	62.192	1.00 40.30	A	0
	ATOM	1097	С	GLU 2	259	17.863	85.132	64.870	1.00 35.71	A	C

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	ATOM	1098	0	GLU A	259	18.700	85.499	65.688	1.00 35.67	A	0
	ATOM	1099	N	ASN A	260	17.114	85.980	64.171	1.00 35.37	A	N
	ATOM	1100	CA	asn a		17.264	87.423	64.308	1.00 33.13	A	C
	ATOM	1101	CB	ASN A		17.209	88.081	62.927	1.00 34.73	A A	С
5	ATOM	1102 1103	CG OD1	ASN A	260 260	18.037 19.087	87.335 86.773	61.893 62.205	1.00 35.58 1.00 37.11	A	C
	ATOM	1103		ASN A	260	17.573	87.340	60.653	1.00 37.65	A	N
	ATOM	1105	C	ASN A	260	16.236	88.073	65.229	1.00 31.26	A	c
	ATOM	1106	Ó	ASN A	260	16.106	89.300	65.261	1.00 34.44	A	0
10	ATOM	1107	N		261	15.494	87.255	65.963	1.00 27.11	A	N
	ATOM	1108	CA	LEU A	261	14.501	87.762	66.902	1.00 24.52 1.00 24.18	A A	C
	ATOM	1109 1110	CB	LEU A	261 261	13.147	87.089 87.443	66.648 65.340	1.00 24.18 1.00 22.90	A	c
	ATOM	1111		LEU A	261	11.116	86.685	65.252	1.00 24.50	A	č
15	ATOM	1112			261	12.172	88.923	65.296	1.00 21.37	A	C
	ATOM	1113	C	LEU A	261	14.986	87.476	68.329	1.00 22.38	A	C
	ATOM	1114	0	PER Y	261	15.179	86.321	68.694	1.00 23.95	A	0
	MOTA	1115	N		262	15.182	88.524 88.370	69.126 70.499	1.00 20.79 1.00 20.67	A A	C
20	ATOM ATOM	1116 1117	CB	LEU A	262	15.670 16.810	89.376	70.758	1.00 20.87	A	č
20	ATOM	1118	CG		262	17.955	89.381	69.723	1.00 21.77	A	č
	ATOM	1119	CD1		262	18.955	90.499	70.035	1.00 21.55	A	С
	ATOM	1120	CD2		262	18.672	88.033	69.723	1.00 20.67	A	С
	ATOM	1121	C		262	14.556	88.538	71.543	1.00 20.45	A	C
25	MOTA MOTA	1122 1123	O N		262 263	13.484 14.820	89.054 88.095	71.232 72.775	1.00 21.30 1.00 19.96	A A	N
	ATOM	1124	CA	LEU A		13.855	88.172	73.875	1.00 20.52	Ã	Ĉ
	ATOM	1125	CB	LEU A		13.556	86.769	74.407	1.00 20.43	A	C
	ATOM	1126	CG	LEU A		12.804	85.816	73.471	1.00 22.66	A	C
30	MOTA	1127	CD1			12.979	84.366	73.956	1.00 21.47	A	C
	ATOM	1128	CD2		263	11.330	86.219	73.415 75.046	1.00 19.52 1.00 22.38	A A	C
	ATOM ATOM	1129 1130	C	LEU A		14.307 15.389	89.045 88.848	75.603	1.00 22.70	A	ŏ
	MOTA	1131	N	GLY A		13.456	89.992	75.429	1.00 21.30	A	N
35	ATOM	1132	CA	GLY A	264	13.765	90.882	76.530	1.00 23.34	A	C
	ATOM	1133	C	GLY A	264	13.574	90.251	77.902	1.00 25.78	A	C
	ATOM	1134	0	GLY A		13.277	89.061	78.025	1.00 24.77	A	O N
	ATOM	1135 1136	N CA	SER A		13.732 13.618	91.067 90.609	78.939 80.321	1.00 27.28	A A	C
40	ATOM	1137	CB	SER A		13.959	91.758	81.270	1.00 29.98	A	č
	ATOM	1138	OG	SER A		14.174	91.285	82.583	1.00 31.27	A	0
	ATOM	1139	С	SER A		12.253	90.039	80.684	1.00 29.23	A	C
	ATOM	1140	0	SER A		12.158	89.086	81.449	1.00 30.53	A A	0
45	ATOM	1141 1142	N CA	ALA A		11.193 9.845	90.623 90.156	80.140 80.432	1.00 29.57 1.00 28.18	A A	C
43	ATOM	1142	CB	ALA A		8.889	91.338	80.475	1.00 28.62	A	č
	ATOM	1144	c	ALA A		9.373	89.141	79.399	1.00 27.11	A	C
	MOTA	1145	0	ALA A		8.211	88.749	79.393	1.00 29.47	A	0
	MOTA	1146	N	GLY A		10.274	88.717	78.524	1.00 25.83	A	N
50	MOTA	1147	CA C	GLY A		9.900 9.343	87.759 88.414	77.502 76.249	1.00 24.74	A A	C
	ATOM ATOM	1148 1149	Ö	GLY A		8.829	87.729	75.365	1.00 22.75	A	ŏ
	ATOM	1150	N	GLU A		9.435	89.740	76.167	1.00 24.05	A	N
	ATOM	1151	. CA	GLU A	268	8.942	90.468	74.993	1.00 25.88	A	С
55	MOTA	1152	CB	GLU A	268	8.748	91.951	75.328	1.00 27.62	A	Č
	ATOM	1153	CG	GLU A	268	8.880 10.323	92.266	76.803 77.243	1.00 33.71 1.00 35.40	A A	C
	ATOM	1154 1155	CD OE1	GLU A	268	10.323	93.537	77.049	1.00 36.57	λ	Ö
	ATOM	1156		GLUA		10.909	91.465	77.773	1.00 36.25	A	ō
60	ATOM	1157	C	GLU A		9.920	90.327	73.820	1.00 24.17	A	C
	ATOM	1158	0	GLU A		11.138	90.213	74.021	1.00 23.37	A	0
	ATOM	1159	N	LEU A		9.380	90.317	72.603	1.00 22.43	A A	U.
	ATOM	1160 1161	CB	LEU A		10.185 9.291	90.189 89.793	71.388 70.204	1.00 22.74 1.00 27.41	A	c
65	ATOM	1162	CG	LEU A		8.740	88.370	70.198	1.00 30.77	A	c
33	ATOM	1163	CD1			7.689	88.219	69.115	1.00 32.33	A	C
	ATOM	1164	CD2	LEU A	269	9.893	87.387	69.981	1.00 30.69	A	C
	ATOM	1165	C	LEU A		10.941	91.466	71.024	1.00 20.79	A	C
70	ATOM	1166 1167	O N	LEU A		10.427 12.164	92.569 91.310	71.176 70.536	1.00 20.86	A A	O N
/0	ATOM	1168	CA	LYS A		12.164	92.453	70.536	1.00 19.86	A	C
	ATOM	1169	CB	LYS Z		14.179	92.628	71.046	1.00 19.41	A	č

							-61-				
	MOTA	1170	CG	LYS	A 27	13.839	92.907	72.512	1.00 21.56	A	С
	ATOM	1171	CD		A 27		94.336	72.739	1.00 21.90	A	ē
	ATOM	1172	CE		A 27		94.578	74.222	1.00 19.95	A	C
_	MOTA	1173	NZ		A 27		96.006	74.509	1.00 19.75	A	N
5	MOTA	1174	С		A 27		92.201	68.703	1.00 19.52	A	C
	MOTA	1175	0		A 27		91.199	68.458	1.00 19.94	A	0
	MOTA	1176 1177	N CA		A 27 A 27		93.092 92.946	67.768 66.388	1.00 20.30 1.00 19.95	A A	N
	MOTA	1178	CB		A 27		93.645	65.375	1.00 19.95	A	c
10	MOTA	1179	CG2		A 27		93.602	63.959	1.00 22.31	A	č
	ATOM	1180	CG1		A 27		92.952	65.349	1.00 23.31	A	č
	ATOM	1181	CD1	ILE	A 27		93.557	64.325	1.00 23.77	A	č
	MOTA	1182	C		A 27	14.966	93.584	66.273	1.00 20.17	A	C
	ATOM	1183	0		A 27		94.761	66.590	1.00 19.60	A	0
15	ATOM	1184	N		A 27		92.805	65.822	1.00 20.80	A	N
	ATOM	1185	CA		A 27		93.291	65.675	1.00 22.55	A	C
	ATOM	1186 1187	CB C		A 27		92.307 93.477	66.319 64.199	1.00 22.63 1.00 23.77	A	C
	ATOM	1188	ŏ		A 27		92.985	63.335	1.00 23.77 1.00 27.69	A A	0
20	ATOM	1189	N		A 27		94.166	63.914	1.00 25.21	A	N
	ATOM	1190	CA	ASP	A 27		94.423	62,535	1.00 26.15	A	Ĉ
	ATOM	1191	CB	ASP	A 27		95.919	62.371	1.00 26.59	A	c
	ATOM	1192	CG	ASP	A 27		96.364	60.922	1.00 28.71	A	C
	ATOM	1193	OD1	ASP	A 27		97.503	60.662	1.00 27.94	A	0
25	ATOM	1194	OD2	ASP	A 27		95.587	60.048	1.00 26.80	A	0
	ATOM	1195 1196	C	ASP	A 27		93.608	62.114	1.00 28.69	A	C
	ATOM	1196	N	PHE	A 27		94.134 92.325	62.036 61.825	1.00 31.16 1.00 31.46	A A	O
	ATOM	1198	CA	PHE	A 27		91.445	61.410	1.00 31.46	A	C
30	ATOM	1199	CB	PHE	A 27		90.005	61.826	1.00 34.86	A	č
	ATOM	1200	CG	PHE	A 27		89.762	63.298	1.00 34.01	A	č
	MOTA	1201	CD1	PHE	A 27	22.369	89.593	63.891	1.00 35.57	A	C
	ATOM	1202	CD2	PHE	A 27		89.690	64.091	1.00 33.84	A	С
25	MOTA	1203	CE1	PHE	A 27		89.352	65.255	1.00 34.13	A	C
35	MOTA MOTA	1204 1205	CE2	PHE	A 27		89.449	65.458	1.00 33.04	A	С
	ATOM	1205	CZ	PHE	A 27		89.279 91.465	66.043 59.908	1.00 35.67 1.00 35.98	A A	C
	ATOM	1207	ŏ	PHE	A 27		91.357	59.508	1.00 37.36	A	Ö
	ATOM	1208	N		A 27		91.607	59.065	1.00 36.77	A	N
40	ATOM	1209	CA	GLY	A 27		91.613	57.640	1.00 38.21	A	c
	ATOM	1210	С		A 27		93.012	57.108	1.00 39.96	A	С
	ATOM	1211	0		A 27		93.371	56.030	1.00 40.54	A	0
	ATOM	1212	N	TRP			93.801	57.850	1.00 40.99	A	N
45	ATOM	1213 1214	CA	TRP			95.178	57.454 58.633	1.00 41.46	A	C
73	ATOM	1214	CG		A 27		95.958 95.435	59.065	1.00 39.82 1.00 39.01	A A	C
	ATOM	1216	CD2		A 27	25.376	95.801	58.523	1.00 38.81	A	č
	ATOM	1217	CE2		A 27		95.024	59.190	1.00 38.69	A	č
	ATOM	1218	CE3		A 27	25.790	96.707	57.538	1.00 38.86	A	C
50	ATOM	1219	CD1		A 27		94.481	60.014	1.00 37.17	A	С
	ATOM	1220	NE1	TRP	A 27		94.231	60.092	1.00 36.72	A	N
	MOTA	1221			A 27		95.125	58.905	1.00 39.22	A	c
	ATOM	1222 1223	CZ3 CH2	TRP			96.809 96.018	57.249 57.934	1.00 40.49 1.00 39.41	A A	c
55	ATOM	1224	C	TRP		23.152	95.244	56.289	1.00 39.41	A	c
	ATOM	1225	ŏ		A 27	23.334	96.307	55.686	1.00 43.44	A	ŏ
	ATOM	1226	N	SER			94.119	55.982	1.00 42.35	A	N
	MOTA	1227	CA	SER	A 27	24.750	94.058	54.887	1.00 43.23	A	C
	ATOM	1228	CB	SER			93.415	55.360	1.00 42.06	A	C
60	ATOM	1229	OG	SER			92.188	56.032	1.00 41.30	A	0
	MOTA	1230	C	SER			93.244	53.736	1.00 44.99	A	С
	MOTA	1231 1232	O N	SER			93.259	52.619 54.593	1.00 46.90	A	0
	ATOM	1232	CA	GLY			85.906 85.530	54.593	1.00 50.58 1.00 50.41	A A	N
65	MOTA	1234	C	GLY			84.405	53.413	1.00 49.78	A	č
	MOTA	1235	ŏ	GLY			84.652	52.215	1.00 49.58	A	ō
	MOTA	1236	N	THR	A 29	18.024	83.166	53.899	1.00 47.99	A	N
	MOTA	1237	CA	THR			82.001	53.036	1.00 45.67	A	C
70	MOTA	1238	CB	THR			80.671	53.833	1.00 46.93	A	C
70	MOTA	1239	OG1		A 29		80.818	55.127	1.00 47.18	A	0
	MOTA	1240 1241	CG2 C	THR	A 29: A 29:		80.279 82.009	53.988 52.318	1.00 45.73	A A	C
	ATOM	TNAT	-	4nn	n 29.	10.504	82.009	52.318	1.00 43.16	A	C

							-62-				
	ATOM	1242	0	THR	A 29	15.604	82.783	52.650	1.00 42.03	A	0
	ATOM	1243	N	PEA	A 29		81.119	51.340	1.00 41.25	A	N
	MOTA	1244	CA	LEU	A 29:	15.194	80.972	50.514	1.00 39.15	A	С
_	MOTA	1245	CB	FEA	A 29:		79.814	49.540	1.00 41.13	A	C
5	MOTA	1246	CG	PEO	A 29		79.815	48.220	1.00 41.33	A	C
	ATOM	1247	CD1	PEO	A 29: A 29:		81.085 78.592	47.436 47.423	1.00 40.19	A A	C
	ATOM	1248 1249	CD2	LEU	A 29		80.750	51.280	1.00 36.22	A	c
	ATOM	1250	ŏ	LEU	A 29		81.287	50.909	1.00 35.72	A	ŏ
10	ATOM	1251	N	ASP	A 29		79.964	52.346	1.00 32.89	A	N
	ATOM	1252	CA	ASP	A 29		79.647	53.150	1.00 31.62	A	С
	ATOM	1253	CB	ASP	A 29		78.945	54.437	1.00 31.49	A	C
	ATOM	1254	CG		A 29		77.452	54.253	1.00 33.23	A	C
	MOTA	1255	OD1		A 29		76.838	55.076	1.00 35.49 1.00 31.43	A A	0
15	ATOM	1256 1257	OD2		A 29 A 29		76.886 80.779	53.299 53.503	1.00 31.43	A	Ċ
	ATOM	1258	C		A 29		80.563	53.556	1.00 28.20	A	ŏ
	ATOM	1259	N		A 29		81.977	53.748	1.00 28.61	A	и
	ATOM	1260	CA		A 29		83.101	54.128	1.00 27.28	A	C
20	ATOM	1261	CB		A 29	12.064	83.814	55.357	1.00 28.14	A	C
	MOTA	1262	CG		A 29		82.871	56.472	1.00 29.60	A	C
	MOTA	1263	CD1	TYR	A 29	13.669	82.192	56.442	1.00 31.65	A	С
	MOTA	1264	CE1		A 29		81.264	57.423	1.00 33.54	A A	C
25	ATOM ATOM	1265 1266	CD2 CE2		A 29 A 29		82.601 81.669	57.522 58.514	1.00 31.90 1.00 32.48	A	c
23	ATOM	1267	CZ		A 29	13.112	81.005	58.454	1.00 35.17	Ä	č
	ATOM	1268	OH		A 29		80.065	59.406	1.00 37.45	A	ō
	ATOM	1269	C		A 29	11.211	84.126	53.032	1.00 26.29	A	C
	ATOM	1270	0	TYR	A 29	10.530	85.117	53.276	1.00 27.19	A	0
30	ATOM	1271	N		A 29	11.732	83.888	51.830	1.00 25.16	A	N
	ATOM	1272	CA		A 29		84.809	50.709	1.00 24.82	A A	C
	ATOM	1273	CB		A 29 A 29		84.607 85.044	49.669 50.075	1.00 24.50 1.00 25.62	A	c
	ATOM	1274 1275	CG	LEU	A 29		84.731	48.952	1.00 21.99	A	č
35	ATOM	1276			A 29		86.535	50.391	1.00 25.81	A	č
	ATOM	1277	c		A 29		84.671	50.019	1.00 22.65	A	C
	ATOM	1278	0	LEU	A 29	9.736	83.565	49.730	1.00 22.45	A	0
	ATOM	1279	N		A 29		85.800	49.730	1.00 21.47	A	N
	ATOM	1280	CD		A 29		87.159	50.187	1.00 22.06	A A	c
40	ATOM ATOM	1281 1282	CA		A 29 A 29		85.782 87.169	49.066 49.380	1.00 21.33 1.00 20.33	A	č
	ATOM	1283	CG		A 29		88.033	49.450	1.00 21.76	A	č
	ATOM	1284	c		A 29		85.479	47.561	1.00 22.16	A	C
	ATOM	1285	0		A 29		85.652	46.917	1.00 19.11	A	0
45	ATOM	1286	N		A 29	7.137	85.032	46.976	1.00 23.42	A	N
	ATOM	1287	CD		A 29		84.826	47.557	1.00 21.93	A	C
	ATOM	1288	CA		A 29		84.720	45.542 45.271	1.00 24.58 1.00 24.85	A A	C
	ATOM	1289 1290	CB		A 29 A 29		84.315 83.791	46.629	1.00 24.85	A	c
50	ATOM	1291	C		A 29		85.869	44.641	1.00 26.51	Ä	č
	ATOM	1292	ŏ		A 29		85.667	43.749	1.00 24.25	A	0
	ATOM	1293	N	GLU	A 29	7.081	87.070	44.884	1.00 28.74	A	N
	MOTA	1294	CA		A 29	7.435	88.231	44.070	1.00 32.43	A	С
	ATOM	1295	CB		A 29		89.508	44.625	1.00 31.92 1.00 31.41	A A	C
55	ATOM	1296 1297	CD		A 29 A 29		89.780 89.259	46.993	1.00 31.41	A	c
	ATOM	1298	OE1		A 29		88.089	46.835	1.00 32.77	A	ŏ
	ATOM	1299	OE2		A 29		90.017	47.864	1.00 32.41	A	ō
	MOTA	1300	C		A 29		88.440	43.934	1.00 34.76	A	C
60	ATOM	1301	0		A 29		88.836	42.872	1.00 34.79	A	0
	MOTA	1302	N		A 29		88.167	45.003	1.00 37.58	A	N
	MOTA	1303	CA		A 29		88.348	44.966	1.00 39.94	A	C
	MOTA	1304	CB	MET	A 29 A 29		88.481 89.800	46.391 47.055	1.00 40.17	A A	C
65	ATOM ATOM	1305 1306	CG	MET	A 29		90.123	48.737	1.00 40.44	A	s
55	ATOM	1306	CE	MET	A 29		90.123	48.365	1.00 41.54	A	c
	ATOM	1308	C	MET			87.268	44.179	1.00 41.00	A	C.
	ATOM	1309	0	MET		9 12.582	87.589	43.237	1.00 42.71	A	0
	ATOM	1310	N	ILE			85.998	44.525	1.00 42.03	A	N
70	ATOM	1311	CA		A 30		84.941	43.784	1.00 43.81	A A	C
	ATOM	1312 1313	CB CG2		A 30		83.535 83.497	44.407 45.829	1.00 44.39	A A	C
	MTOM	1313	CG2	TDE	A 30	12.690	83.497	45.629	1.00 45.06	A	C

							-63-				
	ATOM	1314			A 300	10.656	83.172	44.378	1.00 44.10	A	С
	ATOM	1315	CD1		A 300	10.379	81.745	44.804	1.00 44.41	A	C
	ATOM	1316 1317	C		A 300 A 300	11.906 12.573	84.908 84.322	42.323	1.00 44.98 1.00 45.46	A	C
5	ATOM	1318	N		A 301	10.762	85.529	42.042	1.00 45.85	A A	N
	ATOM	1319	CA		A 301	10.232	85.592	40.682	1.00 46.66	A	C
	ATOM	1320	CB		A 301	8.709	85.477	40.687	1.00 47.45	A	č
	ATOM	1321	CG		A 301	8.189	84.054	40.721	1.00 48.05	A	С
10	ATOM ATOM	1322 1323	CD OE1		A 301 A 301	6.688 5.979	83.997	40.916	1.00 49.14	A	C
10	ATOM	1324	OE2		A 301	6.218	84.782 83.166	40.253	1.00 50.01 1.00 48.90	A A	0
	ATOM	1325	c		A 301	10.643	86.904	40.026	1.00 47.81	A	c
	ATOM	1326	0		A 301	10.048	87.326	39.035	1.00 47.15	A	ō
	ATOM	1327	N		A 302	11.650	87.547	40.613	1.00 49.04	A	N
15	ATOM	1328 1329	CA		A 302	12.193	88.792	40.094	1.00 50.61	A	С
	ATOM	1330	0		A 302 A 302	11.296 11.642	89.991 90.841	39.844 39.025	1.00 51.92 1.00 52.54	A A	C
	ATOM	1331	N		A 303	10.167	90.087	40.542	1.00 52.54	A	N
	ATOM	1332	CA		A 303	9.259	91.219	40.356	1.00 53.57	A	č
20	ATOM	1333	CB		A 303	7.812	90.753	40.529	1.00 55.04	A	C
	ATOM	1334 1335	CD		A 303	7.494	89.500	39.724	1.00 58.17	A	C
	ATOM	1335	NE		A 303 A 303	6.011 5.212	89.149 90.072	39.750 38.947	1.00 60.28 1.00 62.73	A A	C N
	MOTA	1337	CZ		A 303	3.919	89.903	38.680	1.00 63.00	A	C
25	MOTA	1338			A 303	3.271	90.794	37.941	1.00 62.86	Ä	N
	MOTA	1339			A 303	3.275	88.842	39.150	1.00 62.02	A	N
	MOTA	1340	C		A 303	9.571	92.371	41.320	1.00 52.69	A	C
	MOTA	1341 1342	O		A 303 A 304	10.582 8.710	92.344 93.385	42.020 41.344	1.00 52.06 1.00 52.57	A A	N
30	ATOM	1343	CA		A 304	8.907	94.539	42.223	1.00 52.57	A	C
	MOTA	1344	CB		A 304	8.395	95.820	41.542	1.00 55.47	A	c
	MOTA	1345	CG		A 304	8.972	97.135	42.103	1.00 59.08	A	C
	ATOM	1346 1347	SD		A 304	7.948	98.022	43.326	1.00 62.23	A	s
35	ATOM	1347	CE		A 304 A 304	7.208 8.153	99.317 94.299	42.301	1.00 60.78 1.00 51.89	A A	C
	ATOM	1349	ŏ		A 304	7.026	93.809	43.511	1.00 51.03	A	ŏ
	ATOM	1350	N	HIS .	A 305	8.775	94.645	44.651	1.00 50.91	A	N
	ATOM	1351	CA		A 305	8.149	94.441	45.953	1.00 49.66	A	C
40	ATOM	1352 1353	CB		A 305	8.944	93.415	46.762	1.00 51.52	A	C
40	MOTA	1354	CG CD2		A 305 A 305	10.392 11.085	93.763 94.211	46.926 48.000	1.00 54.62 1.00 54.89	A	C
	MOTA	1355			A 305	11.304	93.665	45.897	1.00 55.05	A	N.
	MOTA	1356	CE1	HIS .	A 305	12.496	94.034	46.330	1.00 55.54	A	c
45	MOTA	1357	NE2		A 305	12.391	94.371	47.603	1.00 55.94	A	N
45	MOTA	1358 1359	C		A 305 A 305	7.996 8.620	95.712 96.730	46.778 46.491	1.00 47.80	A	C
	ATOM	1360	N	ASP	A 306	7.150	95.635	47.802	1.00 47.81 1.00 45.38	A A	N
	ATOM	1361	CA	ASP .	A 306	6.903	96.746	48.713	1.00 43.84	À	č
	MOTA	1362	CB		A 306	5.667	97.548	48.278	1.00 44.46	A	C
50	MOTA	1363 1364	CG		A 306	4.424	96.691	48.154	1.00 45.21	A	C
	ATOM	1365		ASP .		4.281	95.727 96.992	48.935 47.285	1.00 45.61 1.00 45.96	A A	0
	ATOM	1366	C		A 306	6.714	96.213	50.141	1.00 42.01	A	c
	ATOM	1367	ō		A 306	7.276	95.181	50.498	1.00 40.43	A	ŏ
55	ATOM	1368	N		A 307	5.917	96.910	50.948	1.00 41.41	A	N
	ATOM	1369	CA	GLU .		5.684	96.503	52.334	1.00 40.47	A	С
	ATOM	1370 1371	CG	GLU .	A 307 A 307	5.047 3.673	97.658 98.084	53.116 52.624	1.00 43.34	A	C
	ATOM	1372	CD		A 307	2.543	97.317	53.287	1.00 53.33	A A	c
60	ATOM	1373		GLU :		1.369	97.561	52.933	1.00 56.15	A	ō
	ATOM	1374	OE2		A 307	2.822	96.475	54.168	1.00 56.15	A	0
	ATOM	1375 1376	C		A 307 A 307	4.838	95.236	52.486	1.00 37.15	A	С
	ATOM	1377	N		A 307	4.595	94.774 94.668	53.603 51.367	1.00 36.77	A A	O N
65	ATOM	1378	CA		A 308	3.599	93.455	51.411	1.00 29.96	A	C
	ATOM	1379	CB		A 308	2.842	93.262	50.095	1.00 31.75	A	C
	ATOM	1380	CG		A 308	1.668	94.214	49.908	1.00 30.26	A	C
	ATOM	1381 1382	CD		A 308 A 308	0.631	94.005	50.994	1.00 30.93	A	C
70	ATOM	1382	NZ		A 308	-0.590 -1.687	94.881 94.574	50.766 51.722	1.00 33.18 1.00 31.42	A A	C
	ATOM	1384	C		A 308	4.452	92.227	51.704	1.00 31.42	A	C
	ATOM	1385	0	LYS		3.918	91.178	52.055	1.00 26.90	A	ŏ

							-64-				
	ATOM	1386 1387	N CA		A 309	5.772	92.354	51.566	1.00 26.12	A	N
	ATOM	1388	CB		A 309 A 309	6.666 8.147	91.230	51.849	1.00 27.15	A	C
	ATOM	1389	CG1		A 309	8.273	91.546 91.828	51.483 49.988	1.00 28.50 1.00 28.82	A	C
5	ATOM	1390	CG2		A 309	8.648	92.728	52.299	1.00 28.82	A	С
	ATOM	1391	C		A 309	6.608	90.885	53.339	1.00 28.83	A A	C
	ATOM	1392	õ		A 309	6.748	89.720	53.725	1.00 27.51	A	0
	ATOM	1393	N		A 310	6.382	91.905	54.167	1.00 25.49	A	N
	ATOM	1394	CA		A 310	6.308	91.715	55.607	1.00 23.57	A	C
10	ATOM	1395	CB		A 310	6.281	93.069	56,332	1.00 23.42	A	č
	ATOM	1396	CG	ASP .	A 310	7.564	93.858	56.139	1.00 26.52	A	č
	ATOM	1397	OD1			8.657	93.249	56.164	1.00 26.12	A	ŏ
	ATOM	1398	OD2	ASP .	A 310	7.489	95.095	55.974	1.00 28.59	A	ō
	ATOM	1399	C		A 310	5.106	90.878	56.012	1.00 21.40	A	Ċ
15	ATOM	1400	0		A 310	5.147	90.193	57.038	1.00 21.03	A	0
	ATOM	1401	N	LEU 2		4.032	90.932	55.228	1.00 20.72	A	N
	ATOM	1402	CA	LEU 2		2.848	90.126	55.541	1.00 20.20	A	C
	ATOM	1403	CB	LEU .		1.628	90.564	54.713	1.00 19.65	A	C
20	ATOM	1404	CG	LEU :		0.794	91.785	55.141	1.00 21.99	A	C
20	ATOM	1405		LEU :		0.255	91.575	56.547	1.00 23.33	A	C
	ATOM	1406		LEU		1.635	93.047	55.092	1.00 23.76	A	C
	ATOM	1407 1408	C	LEU 2		3.171	88.658	55.238	1.00 18.99	A	C
	ATOM	1409	N		A 311	2.764 3.892	87.760	55.960	1.00 16.87	A	0
25	ATOM	1410	CA		A 312	4.284	88.424 87.069	54.148 53.786	1.00 19.04	A	N
23	ATOM	1411	CB		A 312	5.094	87.083	52.482	1.00 19.16 1.00 19.35	A	C
	ATOM	1412	CG	TRP		5.628	85.742	52.102	1.00 19.35	A A	C
	ATOM	1413	CD2		A 312	4.970	84.762	51.294	1.00 17.19	A	C
	ATOM	1414	CE2			5.813	83.629	51.242	1.00 16.50	A	č
30	ATOM	1415	CE3		A 312	3.747	84.730	50.607	1.00 17.90	A	č
	ATOM	1416	CD1		312	6.815	85.184	52.496	1.00 19.08	A	č
	ATOM	1417	NE1			6.933	83.911	51.983	1.00 18.08	A	N
	ATOM	1418	CZ2		A 312	5.473	82.478	50.533	1.00 17.00	A	c
	ATOM	1419	CZ3		A 312	3.409	83.580	49.899	1.00 14.87	A	č
35	ATOM	1420	CH2		A 312	4.271	82.470	49.870	1.00 19.28	A	C
	ATOM	1421	С	TRP 2		5.142	86.497	54.923	1.00 18.64	A	C
	ATOM	1422	0		312	4.883	85.396	55.424	1.00 16.66	A	0
	ATOM	1423	N	SER A		6.154	87.259	55.333	1.00 15.99	A	N
40	ATOM	1424 1425	CA	SER A	313	7.043	86.823	56.408	1.00 18.14	A	С
40	ATOM	1425	OG	SER A		8.034 8.746	87.931	56.760	1.00 18.03	A	c
	ATOM	1427	C	SER 2		6.254	88.320 86.450	55.604	1.00 20.11	A	0
	ATOM	1428	ŏ		1 313	6.538	85.460	57.650 58.303	1.00 15.82 1.00 16.33	A A	C
	ATOM	1429	N	LEU 2		5.251	87.249	57.967	1.00 17.05	A	N
45	ATOM	1430	CA	LEU /		4.429	86.997	59.137	1.00 18.31	A	C
	ATOM	1431	CB		314	3.408	88.136	59.273	1.00 21.36	A	č
	ATOM	1432	CG		314	3.115	88.707	60.664	1.00 25.08	A	č
	ATOM	1433	CD1	LEU 2	314	4.403	89.035	61.393	1.00 26.53	A	č
	ATOM	1434	CD2	LEU 7		2.258	89.954	60.524	1.00 26.95	A	C
50	ATOM	1435	С	LEU A		3.736	85.627	59.044	1.00 17.43	A	C
	ATOM	1436	0	LEU A	314	3.565	84.928	60.046	1.00 16.65	A	0
	ATOM	1437	N	GLY 7	315	3.348	85.242	57.835	1.00 17.42	A	N
	ATOM ATOM	1438 1439	CA	GLY 7	315	2.682	83.961	57.646	1.00 16.42	A	С
55	ATOM	1440	C	GLY A	315	3.623	82.781	57.799	1.00 13.19	A	С
33	ATOM	1441	N	GLY A	315	3.275 4.816	81.775	58.411	1.00 12.24	A	0
	ATOM	1442	CA	VAL A	316	5.810	82.900 81.844	57.231 57.322	1.00 11.93 1.00 12.52	A	N
	ATOM	1443	CB	VAL 2	316	7.085	82.225	56.521	1.00 12.52	A	C
	ATOM	1444		VAL 7		8.233	81.270	56.858	1.00 14.29	A A	c
60	ATOM	1445		VAL 2		6.779	82.186	55.011	1.00 11.86	A	c
	ATOM	1446	c	VAL 2		6.182	81.591	58.784	1.00 15.03	A	č
	ATOM	1447	ō	VAL 7		6.310	80.446	59.213	1.00 17.62	A	ŏ
	MOTA	1448	N	LEU 2		6.343	82.679	59.534	1.00 14.58	A	N
	ATOM	1449	CA	LEU 2	317	6.709	82.651	60.945	1.00 16.47	A	c
65	ATOM	1450	CB	LEU A		7.011	84.077	61.402	1.00 19.62	A	č
	ATOM	1451	CG	LEU A		8.077	84.260	62.478	1.00 23.94	A	C
	ATOM	1452		LEU 2		9.386	83.649	61.992	1.00 23.88	A	C
	MOTA	1453			317	8.256	85.742	62.782	1.00 25.46	A	С
70	MOTA	1454	c	LEU A		5.618	82.058	61.837	1.00 17.53	A	C
/0	ATOM	1455	0	LEU A		5.897	81.270	62.752	1.00 16.69	A	0
	ATOM ATOM	1456 1457	N CA	CYS A		4.371	82.444	61.578	1.00 15.98	A	N
	ALOM	T421	CA	CIP	7 218	3.272	81.937	62.380	1.00 15.13	A	C

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	MOTA	1458	CB	CYS			1.940	82.520	61.898	1.00 13			
	ATOM	1459	SG	CYS			0.563	82.056	62.970	1.00 20			
	MOTA	1460 1461	C	CYS		318	3.253 3.087	80.420 79.710	62.263 63.245	1.00 14		- 1	A C
5	MOTA	1462	N	TYR			3.421	79.942	61.038	1.00 15			A N
-	ATOM	1463	CA	TYR	Ā	319	3.444	78.518	60.742	1.00 15		- 3	
	ATOM	1464	CB	TYR	Α	319	3.583	78.317	59.226	1.00 14			A C
	ATOM	1465	CG	TYR			3.545	76.875	58.766	1.00 14		2	
10	ATOM	1466		TYR			4.651	76.036	58.902	1.00 13		- 4	
10	ATOM ATOM	1467 1468	CE1	TYR			4.612 2.396	74.713	58.446	1.00 16		1	
	ATOM	1469	CE2	TYR			2.345	76.357 75.047	58.167 57.710	1.00 17			y C
	ATOM	1470	CZ	TYR			3.445	74.231	57.849	1.00 16			i č
	ATOM	1471	OH			319	3.363	72.937	57.385	1.00 15			. 0
15	ATOM	1472	C	TYR			4.610	77.831	61.462	1.00 15			r C
	ATOM	1473	0	TYR			4.407	76.869	62.193	1.00 14			٥ 4
	MOTA MOTA	1474 1475	N	GLU			5.828 7.000	78.330 77.734	61.246	1.00 17			A N
	MOTA	1475	CA	GLU			8.281	78.487	61.880 61.507	1.00 17			7 C
20		1477	CG	GLU			9.537	77.819	62.068	1.00 22			a c
	ATOM	1478	CD	GLU			10.838	78.346	61.469	1.00 26		- 2	
	MOTA	1479	OE1				11.904	77.777	61.784	1.00 27		2	
	MOTA	1480	OE2	GLU			10.807	79.319	60.692	1.00 26		2	
25	MOTA	1481 1482	C	GLU			6.845 7.234	77.672 76.689	63.404 64.019	1.00 17			
23	MOTA	1483	N	PHE			6.259	78.702	64.006	1.00 17		2	
	ATOM	1484	CA	PHE			6.057	78.697	65.458	1.00 18		- 2	
	MOTA	1485	CB	PHE			5.387	79.993	65.948	1.00 18	3.10	1	
	ATOM	1486	CG	PHE			6.318	81.180	66.061	1.00 20			A C
30		1487		PHE			7.705	81.017	66.064	1.00 21		2	
	ATOM ATOM	1488 1489		PHE			5.796 8.554	82.472 82.127	66.152 66.150	1.00 20		2	
	ATOM	1490		PHE			6.632	83.587	66.238	1.00 21		- 2	
	ATOM	1491	CZ	PHE	Ã	321	8.013	83.417	66.236	1.00 23		- 2	
35	ATOM	1492	C	PHE			5.174	77.530	65.896	1.00 19		2	
	ATOM	1493	0	PHE			5.466	76.848	66.878	1.00 18		2	
	ATOM	1494 1495	N	LEU			4.089 3.134	77.309	65.159	1.00 18		2	
	ATOM	1495	CB	PEA			1.777	76.258 76.572	65.498 64.859	1.00 18		2	
40	ATOM	1497	CG	LEU			1.016	77.755	65.455	1.00 16		ź	
	ATOM	1498	CD1	LEU	А	322	-0.128	78.162	64.528	1.00 20		,	
	ATOM	1499		LEU			0.490	77.372	66.833	1.00 14		2	. C
	ATOM	1500	С	LEU			3.530	74.833	65.136	1.00 17		2	
45	MOTA	1501 1502	O N	LEU			3.286 4.138	73.908 74.670	65.908 63.963	1.00 15		2	
43	ATOM	1502	CA	VAL			4.138	73.360	63.462	1.00 17		2	
	ATOM	1504	CB	VAL			4.441	73.318	61.909	1.00 19		1	
	ATOM	1505	CG1	VAL			4.742	71.915	61.399	1.00 21		2	C C
	MOTA	1506		VAL			3.069	73.746	61.462	1.00 18		2	r c
50	ATOM	1507 1508	C	VAL			5.934	72.926	63.890	1.00 19		2	
	ATOM	1508	O N	VAL	Α	324	6.164 6.865	71.746 73.873	64.148 63.975	1.00 18		2	
	ATOM	1510	CA	GLY	Ã	324	8.218	73.524	64.380	1.00 19		,	
	ATOM	1511	C	GLY	А	324	9.219	73.717	63.257	1.00 21	.90	2	
55	ATOM	1512	0	GLY			10.429	73.731	63.486	1.00 23		2	
	ATOM	1513	N	LYS			8.715	73.851	62.034	1.00 23		2	
	ATOM	1514 1515	CA	LYS			9.560 10.035	74.078 72.748	60.873 60.282	1.00 23		2	
	ATOM	1516	CG	LYS			8.940	71.860	59.738	1.00 28		2	
60	ATOM	1517	CD	LYS			9.550	70.690	58.988	1.00 31		,	
	ATOM	1518	CE	LYS			8.492	69.716	58.508	1.00 32	.54	I	. C
	ATOM	1519	NZ	LYS			7.811	69.057	59.655	1.00 36	.73	I	
	ATOM	1520	C	LYS			8.775	74.886	59.838	1.00 22	. 65	7	
65	ATOM	1521 1522	O N	LYS			7.546 9.480	74.928 75.543	59.884 58.897	1.00 20		2	
55	ATOM	1523	CD	PRO			10.936	75.420	58.702	1.00 21		,	
	ATOM	1524	CA	PRO	А	326	8.891	76.368	57.836	1.00 21		2	C C
	ATOM	1525	CB	PRO			10.118	76.980	57.165	1.00 23	.22	7	C
70	ATOM	1526	CG	PRO			11.115	75.882	57.275	1.00 22		7	, C
70	ATOM	1527 1528	C	PRO			8.000	75.589	56.865	1.00 19		I	
	ATOM	1528	N	PRO			8.191 7.015	74.391 76.272	56.637 56.266	1.00 17		7	
		1000							0000	T.00 TO			- 44

	ATOM	1530	CD	PRO	A 32	7 6.590	- 66- 77 - 659	56.535	1 00	18.59	A	c
	ATOM	1531	CA		A 32		75.600	55.336	1.00	19.17	A	
	ATOM	1532	CB		A 32		76.594	55.212	1.00	19.31	A	
5	ATOM	1533	CG		A 32		77.918	55.424		21.80	A	C
3	ATOM	1534 1535	C		A 32		75.105	53.976		20.25	A	
	ATOM	1536	N		A 32		74.185 75.672	53.412 53.449	1.00	22.68	A	
	ATOM	1537	CA		A 32		75.244	52.134	1.00		A A	
	ATOM	1538	CB		A 32		76.469	51.220	1.00		A	
10		1539	CG		A 32		77.331	51.119	1.00		A	
	ATOM	1540		PHE			76.903	50.385	1.00		A	C
	ATOM	1541 1542	CD2	. DHE			78.561	51.776	1.00		A	
	ATOM	1542	CE2		A 32 A 32		77.688 79.354	50.307	1.00		A	
15	ATOM	1544	CZ		A 32		78.912	51.709 50.967		20.03 18.39	A A	
	ATOM	1545	c		A 32		74.466	52.163		24.45	A	
	MOTA	1546	0		A 32	8 10.149	74.296	51.131		24.06	A	
	MOTA	1547	И		A 32		73.992	53.337		26.19	A	N
20	MOTA MOTA	1548	CA		A 32		73.255	53.465	1.00	28.35	A	
20	ATOM	1549 1550	CG		A 32 A 32		72.938	54.936		31.29	A	C
	ATOM	1551	CD		A 32		72.478 71.963	55.236 56.648		37.80 41.63	A	C
	ATOM	1552	OE1		A 32		70.880	56.938		41.71	A A	C
	ATOM	1553	OE2		A 32		72.646	57.468		44.04	Ā	ŏ
25	ATOM	1554	C		A 32		71.955	52.647	1.00	27.64	A	C
	ATOM	1555	0		A 32		71.193	52.639		25.94	A	0
	ATOM ATOM	1556 1557	N		A 33 A 33		71.714	51.962	1.00	26.33	A	N
	ATOM	1558	CB		A 33		70.507 70.731	51.149 49.731	1.00	28.04 25.92	A	C
30	ATOM	1559	c		A 33		70.099	51.084	1 00	28.74	A A	C
	MOTA	1560	ō		A 33		70.838	51.537		29.37	A	ŏ
	MOTA	1561	N		A 33		68.930	50.513		30.23	A	N
	MOTA	1562	CA		A 33		68.421	50.411		31.60	A	C
35	ATOM ATOM	1563 1564	CB		A 33 A 33		66.949	50.002		34.66	A	Ċ
55	ATOM	1565	OD1		A 33		66.069 65.949	51.041 52.165		38.24	A A	C
	ATOM	1566	ND2		A 33		65.449	50.672		42.35	A	N
	MOTA	1567	C	ASN	A 33	16.532	69.189	49.459		31.72	Ã	č
40	MOTA	1568	0		A 33		69.115	49.572	1.00	31.03	A	ō
40	MOTA	1569	N		A 33		69.918	48.512		31.48	A	N
	ATOM ATOM	1570 1571	CA		A 33 A 33		70.684 70.011	47.566		29.77	A	C
	ATOM	1572	OG1		A 33		70.011	46.173 45.606		28.89	A A	0
	ATOM	1573	CG2		A 33		68.580	46.279		27.84	A	C
45	ATOM	1574	C		A 33	16.270	72.118	47.383		31.57	A	č
	ATOM	1575	0		A 33		72.433	47.603		30.47	A	0
	ATOM	1576 1577	CA		A 33		72.981	46.990		30.46	A	N
	ATOM	1578	CB		A 33 A 33		74.386 75.094	46.744		32.40	A A	C
50	ATOM	1579	CG		A 33		75.216	47.286		39.94	A	C
	MOTA	1580	CD1	TYR	A 33	20.620	75.025	46.934		41.64	A	č
	MOTA	1581	CE1	TYR			75.157	47.874		43.08	A	C
	MOTA	1582	CD2 CB2	TYR	A 33	18.992	75.542	48.608		40.76	A	C
55	ATOM	1583 1584	CE2	TYR	A 33		75.677	49.555		43.70	A	C
55	ATOM	1585	OH		A 33		75.483 75.613	49.178 50.107		43.66 47.82	A	C
	ATOM	1586	c		A 33		74.529	45.671		31.07	A A	č
	ATOM	1587	0		A 33	14.916	75.327	45.807		31.04	A	ŏ
	ATOM	1588	34		A 33		73.754	44.601		29.99	A	164
60	ATOM	1589	CA		A 33		73.778	43.471		30.74	A	C
	ATOM	1590 1591	CB	GLN	A 33	15.526 14.434	72.779 72.304	42.403		33.77	A	C
	ATOM	1592	CD	GLM	A 33	13.963	73.367	41.439		41.43	A	C
	ATOM	1593	OE1	GLN	A 33	13.366	74.388	40.820		47.38	A A	0
65	MOTA	1594	NE2	GLN	A 334	14.222	73.120	39.156		47.54	A	N
	ATOM	1595	c		A 33		73.480	43.878	1.00	27.78	A	C
	MOTA	1596 1597	O N		A 334		74.204	43.504	1.00	26.99	A	0
	MOTA	1597	CA		A 33! A 33!		72.412 72.041	44.641	1.00	26.65	A	N
70	ATOM	1599	CB		A 33		70.678	45.085 45.785		26.25	A A	c
	ATOM	1600	CG		A 335		70.193	46.294		34.80	A A	c
	ATOM	1601	CD	GLU .	A 335		70.092	45.197		39.80	A	č

							-67-				
	ATOM	1602			A 335	8.569	69.866	45.539	1.00 41.99	A	0
	ATOM	1603	OE2		A 335	10.101	70.231	43.999	1.00 40.49	A	0
	ATOM	1604	C		A 335	11.502	73.108	46.005	1.00 23.81	A	C
	ATOM	1605	0		A 335	10.295	73.333	45.969	1.00 22.15	A	N
5	MOTA	1606 1607	N CA		A 336 A 336	12.332 11.835	73.781 74.821	46.802 47.710	1.00 21.23 1.00 21.06	A	C
	ATOM	1607	CB	THE	A 336	12.911	75.253	48.723	1.00 20.94	A	č
	ATOM	1609	OG1		A 336	13.207	74.155	49.593	1.00 21.30	A	ŏ
	ATOM	1610	CG2		A 336	12.418	76.430	49,561	1.00 19.68	A	č
10	ATOM	1611	C		A 336	11.375	76.036	46.920	1.00 21.05	A	C
	ATOM	1612	0	THR	A 336	10.317	76.634	47.204	1.00 19.51	A	0
	MOTA	1613	N		A 337	12.177	76.386	45.921	1.00 22.32	A	N
	ATOM	1614	CA		A 337	11.888	77.500	45.026	1.00 23.61	A	C
15	ATOM	1615	CB		A 337	12.987 12.727	77.601 78.643	43.959 42.890	1.00 28.60 1.00 35.53	A A	C
13	ATOM	1616 1617	CG		A 337 A 337	13.096	79.978	43.076	1.00 38.47	A	c
	ATOM	1618	CE1		A 337	12.825	80.947	42.100	1.00 41.00	A	č
	ATOM	1619	CD2		A 337	12.081	78.298	41.700	1.00 38.75	A	c
	ATOM	1620	CE2		A 337	11.803	79.251	40.722	1.00 41.63	A	C
20	ATOM	1621	CZ		A 337	12.177	80.573	40.927	1.00 43.73	A	С
	ATOM	1622	OH		A 337	11.890	81.513	39.958	1.00 46.53	A	0
	ATOM	1623	C		A 337	10.546	77.221	44.346	1.00 22.77	A	C
	ATOM	1624	0	TYR	A 337 A 338	9.680 10.384	78.096 75.988	44.261	1.00 20.90 1.00 22.05	A A	N O
25	ATOM	1625 1626	N CA		A 338	9.163	75.578	43.183	1.00 24.06	A	C
23	ATOM	1627	CB		A 338	9.314	74.153	42.633	1.00 28.55	A	č
	ATOM	1628	CG		A 338	8.183	73.729	41.703	1.00 35.30	A	C
	ATOM	1629	CD		A 338	8.152	72.221	41.440	1.00 41.29	A	C
	ATOM	1630	CE		A 338	9.451	71.691	40.831	1.00 42.96	A	С
30	ATOM	1631	NZ		A 338	10.551	71.612	41.836	1.00 45.52	A	N
	ATOM	1632	C		A 338	7.934	75.656	44.094	1.00 22.36	A A	C
	ATOM ATOM	1633 1634	N O		A 338 A 339	6.894 8.056	76.160 75.174	43.686 45.328	1.00 22.23	A	И
	ATOM	1635	CA		A 339	6.936	75.214	46.263	1.00 19.98	A	Č
35	ATOM	1636	CB		A 339	7.252	74.388	47.506	1.00 21.06	A	č
	ATOM	1637	CG		A 339	7.288	72.892	47.250	1.00 24.15	A	C
	ATOM	1638	CD		A 339	7.637	72.141	48.504	1.00 25.25	A	C
	ATOM	1639	NE		A 339	7.821	70.720	48.241	1.00 30.16	A	N
40	MOTA	1640	CZ		A 339	8.053	69.811	49.182	1.00 30.16	A	C
40	ATOM ATOM	1641 1642			A 339 A 339	8.126 8.217	70.173 68.541	50.456 48.848	1.00 31.69 1.00 32.15	A A	N
	ATOM	1643	C		A 339	6.516	76.626	46.685	1.00 17.94	A	C
	ATOM	1644	ŏ		A 339	5.339	76.878	46.919	1.00 14.93	A	ŏ
	ATOM	1645	N		A 340	7.478	77.536	46.788	1.00 17.04	A	N
45	ATOM	1646	CA		A 340	7.187	78.908	47.175	1.00 16.76	A	C
	ATOM	1647	CB		A 340	8.497	79.705	47.480	1.00 14.52	A	C
	ATOM	1648	CG2		A 340	8.203	81.199 79.209	47.598 48.786	1.00 14.90 1.00 14.96	A A	c
	ATOM	1649 1650	CD1		A 340 A 340	9.127 10.491	79.209	49.095	1.00 14.96	A	c
50	ATOM	1651	CDI		A 340	6.433	79.573	46.030	1.00 16.16	A	č
	ATOM	1652	ō		A 340	5.369	80.139	46.225	1.00 16.78	A	ō
	ATOM	1653	N		A 341	6.988	79.469	44.829	1.00 18.02	A	N
	MOTA	1654	CA		A 341	6.397	80.061	43.636	1.00 19.89	A	C
	ATOM	1655	CB		A 341	7.302	79.792	42.423	1.00 22.71	A	C
55	ATOM	1656	OG		A 341 A 341	6.820 4.982	80.457 79.552	41.269	1.00 27.61 1.00 19.31	A A	0
	ATOM	1657 1658	C		A 341	4.118	80.318	42.946	1.00 18.97	A	ŏ
	ATOM	1659	N		A 342	4.753	78.262	43.594	1.00 19.76	Ã	N
	ATOM	1660	CA		A 342	3.443	77.658	43.382	1.00 21.30	A	c
60	ATOM	1661	CB		A 342	3.597	76.214	42.911	1.00 24.17	A	C
	MOTA	1662	CG		A 342	4.204	76.121	41.531	1.00 26.81	A	C
	MOTA	1663	CD		A 342	4.268	74.702	41.017	1.00 31.06	A	C
	ATOM	1664	NE		A 342	4.686	74.692	39.617	1.00 35.62	A	N
65	MOTA MOTA	1665 1666	CZ		A 342 A 342	4.769 5.157	73.601 73.700	38.868 37.606	1.00 36.48 1.00 40.12	A A	C
0.5	ATOM	1667	NH2		A 342	4.471	72.414	39.382	1.00 38.88	A	N
	ATOM	1668	C		A 342	2.580	77.690	44.634	1.00 21.34	A	Ĉ
	ATOM	1669	0	ARG	A 342	1.403	77.298	44.600	1.00 21.22	A	0
	MOTA	1670	N	VAL	A 343	3.173	78.165	45.729	1.00 19.64	A	N
70	ATOM	1671	CA		A 343	2.499	78.260	47.022	1.00 19.20	A	C
	ATOM	1672	CB		A 343 A 343	1.386	79.323	47.000	1.00 18.65	A	C
	ATOM	1673	CGI	VAL	A 343	0.848	79.534	48.417	1.00 15.93	A	C

							-68-				
	ATOM	1674	CG2	VAL A		1.920	80.622	46.410	1.00 17.93	A	C
	ATOM	1675 1676	c o	VAL A		1.887	76.917 76.793	47.403 47.569	1.00 19.26 1.00 19.70	A A	C
	ATOM	1677	N	GLU A		2.747	75.916	47.544	1.00 17.68	A	N
5	ATOM	1678	CA	GLU A		2.311	74.568	47.879	1.00 19.81	A	Ĉ
	ATOM	1679	CB	GLU A		2.860	73.584	46.830	1.00 19.99	A	č
	ATOM	1680	CG	GLU A		2.339	73.871	45.426	1.00 26.77	A	C
	MOTA	1681	CD	GLU A		3.088	73.125	44.328	1.00 29.54	A	C
	ATOM	1682	OE1	GLU A		2.646	73.198	43.163	1.00 33.31	A	0
10	ATOM	1683	OE2	GLU A		4.115	72.476 74.142	44.619	1.00 30.95	A	0
	ATOM	1684 1685	C	GLU A		2.738 3.928	73.915	49.277 49.529	1.00 19.23	A A	C
	ATOM	1686	N	PHE A		1.763	74.038	50.184	1.00 17.01	A	N
	ATOM	1687	CA	PHE A		2.030	73.621	51.555	1.00 19.56	A	ĉ
15	ATOM	1688	CB	PHE A		2.529	74.811	52,410	1.00 18.38	A	č
	ATOM	1689	CG	PHE A	345	1.461	75.833	52.734	1.00 18.52	A	C
	MOTA	1690		PHE A	345	0.592	75.644	53.810	1.00 21.05	A	C
	ATOM	1691		PHE A		1.313	76.982	51.951	1.00 18.65	A	C
20	MOTA	1692		PHE A		-0.415	76.584	54.102	1.00 16.74	A	C
20	ATOM	1693 1694	CE2	PHE A		0.310 -0.553	77.925 77.720	52.235 53.317	1.00 19.55 1.00 18.36	A	C
	ATOM	1695	C	PHE A	345	0.779	73.033	52.185	1.00 20.33	A	c
	ATOM	1696	ŏ	PHE A	345	-0.332	73.277	51.708	1.00 20.11	A	ŏ
	MOTA	1697	N	THR A		0.969	72.260	53.255	1.00 19.73	A	N
25	ATOM	1698	CA	THR A	346	-0.136	71.655	53.985	1.00 19.58	A	С
	MOTA	1699	CB	THR A	346	-0.326	70.158	53.615	1.00 20.72	A	C
	ATOM	1700	OG1	THR A		0.916	69.459	53.746	1.00 20.60	A	0
	MOTA	1701		THR A	346	-0.821	70.023	52.177	1.00 20.25	A	C
30	ATOM	1702 1703	C	THR A	346	0.116 1.232	71.792 72.103	55.487 55.902	1.00 20.13 1.00 18.25	A A	C
50	ATOM	1704	N	PHE A		-0.932	71.567	56.282	1.00 20.15	A	N
	ATOM	1705	CA	PHE A	347	-0.887	71,673	57.746	1.00 20.73	A	c
	MOTA	1706	CB	PHE A	347	-2.084	72.476	58.280	1.00 19.55	A	C
	MOTA	1707	CG	PHE A		-2.217	73.870	57.720	1.00 20.41	A	С
35	ATOM	1708	CD1	PHE A	347	-1.433	74.909	58.201	1.00 17.74	A	C
	ATOM	1709	CD2	PHE A	347	-3.178	74.150	56.744	1.00 20.45	A	C
	ATOM	1710 1711		PHE A		-1.597 -3.354	76.204 75.449	57.732 56.264	1.00 18.97 1.00 19.38	A A	C
	ATOM	1712	CZ	PHE A		-2.566	76.476	56.757	1.00 20.54	A	c
40	ATOM	1713	C	PHE A	347	-0.983	70.309	58.430	1.00 22.46	Â	č
	ATOM	1714	ō	PHE A		-1.685	69.416	57.952	1.00 21.99	A	ō
	ATOM	1715	N	PRO A	348	-0.285	70.133	59.565	1.00 24.54	A	N
	ATOM	1716	CD	PRO A		0.801	70.979	60.093	1.00 25.31	A	C
40	ATOM	1717	CA	PRO A	348	-0.354	68.854	60.286	1.00 23.76	A	C
45	ATOM	1718 1719	CB	PRO A	348	0.728 1.715	68.991 69.961	61.354 60.728	1.00 24.65 1.00 26.35	A A	C
	ATOM	1720	c	PRO A		-1.756	68.822	60.910	1.00 24.94	A	č
	ATOM .	1721	ŏ	PRO A		-2.389	69.868	61.056	1.00 22.13	A	ŏ
	ATOM	1722	N	ASP A	349	-2.231	67.640	61.286	1.00 27.34	A	N
50	ATOM	1723	CA	ASP A		-3.568	67.503	61.870	1.00 30.19	A	С
	ATOM	1724	CB	ASP A		-3.856	66.047	62.234	1.00 33.25	A	C
	ATOM	1725	CG	ASP A	349	-3.804	65.139	61.045	1.00 37.28	A	C
	MOTA	1726 1727		ASP A		-4.341 -3.232	65.526 64.034	59.987 61.172	1.00 39.75 1.00 41.94	A A	00
55	ATOM	1728	C	ASP A		-3.856	68.342	63.103	1.00 30.17	A	č
	ATOM	1729	ŏ	ASP A		-4.987	68.777	63.293	1.00 29.70	A	ŏ
	ATOM	1730	N	PHE A		-2.855	68.565	63.949	1.00 28.31	A	N
	MOTA	1731	CA	PHE A	350	-3.100	69.334	65.160	1.00 26.49	A	C
	MOTA	1732	CB	PHE A		-1.977	69.094	66.184	1.00 25.79	A	C
60	ATOM	1733	CG	PHE A		-0.600	69.470	65.705	1.00 24.86	A	C
	MOTA	1734 1735	CD1	PHE A		-0.183 0.294	70.798	65.703 65.296	1.00 27.41	A A	C
	ATOM	1736	CE1	PHE A		1.112	68.492 71.143	65.302	1.00 22.65 1.00 23.41	A A	C
	ATOM	1737		PHE A		1.586	68.824	64.895	1.00 23.41	A	č
65	ATOM	1738	CZ	PHE A		1.995	70.153	64.899	1.00 23.36	Ã	č
	ATOM	1739	C	PHE A	350	-3.349	70.830	64.963	1.00 26.28	A	C
	ATOM	1740	0	PHE A		-3.926	71.482	65.833	1.00 26.14	A	0
	ATOM	1741	N	VAL A		-2.957	71.380	63.820	1.00 24.56	A	N
70	ATOM	1742	CA	VAL A		-3.174	72.809	63.600	1.00 23.91	A	C
70	MOTA	1743 1744	CB CG1	VAL A		-2.429 -2.624	73.304	62.341 62.184	1.00 21.91 1.00 22.59	A	C
	ATOM	1745		VAL A		-2.624	74.803	62.184	1.00 22.59	A A	C
	222014	2,43	0.02	TARRET P		0.543	,2.565	02.433	1.00 15.75		_

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	ATOM	1746	C	VAL	А	351	-4.666	73.183	63.510	1.00 23.38	A	С
	ATOM	1747	0	VAL	Α	351	-5.408	72.635	62.707	1.00 23.52	A	ō
	ATOM	1748	N	THR			-5.076	74.123	64.358	1.00 23.53	A	N
_	ATOM	1749	CA	THR			-6.454	74.618	64.463	1.00 24.90	A	C
5	ATOM	1750	CB	THR			-6.561	75.531	65.724	1.00 26.17	A	C
	ATOM ATOM	1751 1752	OG1 CG2	THR			-6.461 -7.872	74.713	66.893	1.00 29.32	A A	o C
	ATOM	1753	C	THR			-7.872 -7.013	76.284 75.350	65.769 63.230	1.00 31.36 1.00 23.73	A A	c
	ATOM	1754	ö	THR			-6.270	75.946	62.447	1.00 23.73	A.	Ö
10	ATOM	1755	N	GLU			-8.335	75.306	63.059	1.00 24.62	Ä	N
	ATOM	1756	CA	GLU			-8.967	75.954	61.909	1.00 24.68	A	c
	ATOM	1757	CB	GLU			-10.468	75.643	61.869	1.00 29.50	A	C
	ATOM	1758	CG	GLU			-10.797	74.232	61.368	1.00 35.19	A	C
15	ATOM	1759	CD	GLU			-10.272	73.983	59.966	1.00 38.71	A	C
13	ATOM	1760 1761	OE1	GLU			-10.401	74.895	59.117 59.703	1.00 40.65	A	0
	ATOM	1762	C	GLU			-9.739 -8.752	72.879 77.464	61.858	1.00 40.38 1.00 21.70	A A	o c
	ATOM	1763	ŏ	GLU			-8.583	78.041	60.782	1.00 19.58	Ä	õ
	ATOM	1764	N	GLY			-8.755	78.106	63.017	1.00 19.06	A.	N
20	ATOM	1765	CA	GLY			-8.551	79.542	63.035	1.00 17.79	A	С
	ATOM	1766	С	GLY			-7.128	79.867	62.603	1.00 18.40	A	C
	ATOM	1767	0	GPA			-6.878	80.874	61.930	1.00 16.97	A	0
	ATOM	1768	N CA	ALA			-6.191	79.009	62.993	1.00 14.57	A	N
25	ATOM ATOM	1769 1770	CB	ALA ALA			-4.794 -3.919	79.210 78.229	62.648 63.439	1.00 15.46 1.00 16.64	A A	C
20	ATOM	1771	c	ALA			-4.589	79.038	61.136	1.00 14.00	A A	c
	ATOM	1772	ŏ	ALA			-3.846	79.800	60.508	1.00 10.53	A.	ŏ
	ATOM	1773	N	ARG	Α	356	-5.269	78.043	60.565	1.00 15.01	A	N
	MOTA	1774	CA	ARG			-5.199	77.759	59.133	1.00 16.46	A	C
30	ATOM	1775	CB	ARG			-6.010	76.503	58.799	1.00 16.70	A	С
	MOTA	1776	CG	ARG			-5.460	75.229	59.389	1.00 18.49	A.	C
	ATOM ATOM	1777 1778	CD	ARG			-6.495 -6.108	74.120 73.006	59.378 58.518	1.00 22.62	A.	C
	ATOM	1779	CZ	ARG			-5.911	71.762	58.945	1.00 28.84	A A	C
35	ATOM	1780		ARG			-6.058	71.463	60.224	1.00 27.32	A.	N
	ATOM	1781		ARG		356	-5.577	70.811	58.086	1.00 31.07	A	N
	ATOM	1782	C	ARG	A	356	-5.758	78.941	58.350	1.00 15.08	A	C
	ATOM	1783	0	ARG		356	-5.225	79.335	57.319	1.00 14.99	A	0
40	ATOM	1784	N	ASP		357	-6.841	79.508	58.860	1.00 18.02	A	N
40	ATOM ATOM	1785 1786	CA	ASP		357 357	-7.466 -8.694	80.646 81.096	58.214 58.994	1.00 18.90	A A	C
	MOTA	1787	CG	ASP		357	-9.406	82.240	58.312	1.00 22.28	A.	č
	ATOM	1788		ASP			-9.966	81.992	57.235	1.00 22.61	A	ŏ
	MOTA	1789		ASP		357	-9.388	83.381	58.830	1.00 24.45	A	0
45	MOTA	1790	С	ASP		357	-6.494	81.824	58.092	1.00 19.94	A.	С
	MOTA	1791	0	ASP		357	-6.289	82.342	56.998	1.00 20.32	A.	0
	ATOM ATOM	1792 1793	N CA	LEU		358	-5.900	82.238	59.211	1.00 18.05	A	N
	ATOM	1794	CB	LEU		358	-4.942 -4.411	83.358 83.613	59.219 60.638	1.00 18.23	A A	c
50		1795	CG	LEU		358	-3.394	84.760	60.758	1.00 20.75	A.	č
	ATOM	1796	CD1	LEU	A	358	-4.012	86.056	60.216	1.00 19.09	A	c
	ATOM	1797		LEU		358	-2.964	84.934	62.208	1.00 17.47	A	C
	ATOM	1798	C	PEA			-3.749	83.145	58.290	1.00 16.19	A.	C
55	ATOM ATOM	1799 1800	O N	LEU		358 359	-3.413 -3.119	84.021 81.983	57.481 58.415	1.00 16.52 1.00 15.38	A	N
55	ATOM	1801	CA	ILE		359	-1.956	81.629	57.613	1.00 15.38	A A	C
	ATOM	1802	CB	ILE		359	-1.329	80.296	58.114	1.00 16.35	A.	č
	ATOM	1803	CG2			359	-0.186	79.879	57.193	1.00 13.83	A	č
	ATOM	1804	CG1	ILE	Α	359	-0.825	80.469	59.553	1.00 17.25	A.	C
60	ATOM	1805		IFE		359	-0.321	79.200	60.220	1.00 14.18	A	C
	ATOM	1806	C	ILE		359	-2.255	81.518	56.112	1.00 17.80	A	С
	ATOM	1807 1808	O N	SER		359 360	-1.398 -3.464	81.829 81.079	55.294	1.00 18.14	A	0
	ATOM	1808	CA	SER			-3.464	80.938	55.759 54.354	1.00 19.68	A	N
65	ATOM	1810	CB	SER		360	-5.153	80.099	54.233	1.00 19.64	A A	č
0.5	ATOM	1811	OG	SER			-4.950	78.757	54.649	1.00 20.82	A.	ŏ
	ATOM	1812	C	SER	A	360	-4.105	82.303	53.714	1.00 22.33	A	C
	ATOM	1813	0	SER			-3.958	82.467	52.501	1.00 20.61	A	0
70	ATOM	1814	N	ARG			-4.500	83.274	54.533	1.00 23.60	A	N
70	ATOM	1815	CA CB	ARG			-4.741	84.633	54.059	1.00 23.75	A.	C
	ATOM	1816 1817	CB	ARG			-5.587 -7.078	85.410 85.081	55.072 55.087	1.00 28.01	A A	C
	,	1011	CG	(0	••	551	-7.076	03.001	33.007	1.00 32.71	n.	-

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	ATOM	1818	CD	ARG			-7.726	85.333	53.723		39.20	A.	C
	ATOM	1819	NE CZ	ARG	A	361	-7.187	86.514	53.042 53.456		44.85	A A	N C
	MOTA	1820 1821		ARG ARG	A	301	-7.332 -8.012	87.772 88.048	54.562		45.54	A.	N
5	ATOM	1822	MHS	ARG	2	361	-6.772	88.759	52.767		47.53	A.	N
_	ATOM	1823	C	ARG	Ã	361	-3.414	85.369	53.863		21.60	A.	c
	ATOM	1824	ō	ARG	A	361	-3.268	86.174	52.941		24.02	A	0
	ATOM	1825	N	LEU	А	362	-2.450	85.078	54.730		19.99	A	N
	ATOM	1826	CA	LEU	Α	362	-1.139	85.730	54.683		18.01	A	С
10	ATOM	1827	CB	LEU			-0.431	85.627	56.042	1.00	15.49	A.	С
	ATOM	1828	CG	LEU			-0.993	86.459	57.207		15.69	A.	c
	ATOM	1829		LEU			-0.312	86.063 87.948	58.496 56.941	1.00	10.97 15.65	A. A	c
	ATOM	1830 1831	CD2	LEU			-0.801 -0.225	85.192	53.603		18.43	a A	c
15	ATOM	1832	ŏ	LEU			0.608	85.930	53.080		18.21	A	ŏ
	ATOM	1833	N	LEU			-0.362	83.911	53.271		19.92	A	N
	ATOM	1834	CA	LEU			0.483	83.328	52.235		21.77	A	С
	ATOM	1835	CB	LEU			0.918	81.910	52.623		21.94	A	C
	ATOM	1836	CG	LEU			1.412	81.704	54.065		26.68	A	С
20	ATOM	1837		LEU			2.276	80.444	54.158		23.94	A	C
	ATOM	1838		LEU			2.215	82.925	54.518		26.76	A	C
	ATOM ATOM	1839 1840	C	LEU			-0.243 -0.570	83.314 82.261	50.892 50.359		22.91 24.15	A A	0
	ATOM	1841	N	LYS			-0.505	84.508	50.370		23.56	A.	N
25		1842	CA	LYS			-1.180	84.691	49.090		23.34	A.	c
	ATOM	1843	CB	LYS			-2.211	85.818	49.181		24.62	A	С
	ATOM	1844	CG	LYS			-3.545	85.423	49.806		26.87	A	C
	ATOM	1845	CD	LYS			-4.289	84.446	48.912		29.10	A	C
	ATOM	1846	CE	LYS			-5.713	84.208	49.392		32.69	A	С
30	ATOM	1847	NZ	LYS	Α	364	-6.503	83.427	48.391		32.47	A	N
	ATOM	1848	c	LYS			-0.144	85.052	48.032		22.89	A	C
	ATOM	1849 1850	O N	HIS			0.696 -0.210	85.929 84.375	48.247 46.893		23.81	A A	N
	ATOM	1851	CA	HIS			0.717	84.624	45.797		23.97	A.	C
35	ATOM	1852	CB	HIS			0.380	83.734	44.602		24.15	A	č
	ATOM	1853	CG	HIS			1.275	83.955	43.426		25.26	A.	č
	ATOM	1854	CD2	HIS	Α	365	1.097	84.673	42.293	1.00	26.54	A	C
	ATOM	1855		HIS			2.563	83.470	43.372		27.83	A	N
	ATOM	1856		HIS			3.142	83.883	42.258	1.00	26.33	A	C
40	ATOM	1857		HIS			2.274	84.617	41.588	1.00	26.94	A	N
	ATOM	1858 1859	C	HIS			0.703 1.757	86.085 86.695	45.354 45.187		24.80	A A	C
	ATOM	1860	N	ASN			-0.491	86.631	45.144		25.39	A.	N
	ATOM	1861	CA	ASN			-0.667	88.027	44.729		28.27	A.	c
45	ATOM	1862	CB	ASN			-2.058	88.197	44.101		30.44	A	C
	ATOM	1863	CG	ASN			-2.331	89.620	43.624		33.56	A	C
	MOTA	1864		ASN			-3.386	89.895	43.051		36.17	A	0
	MOTA	1865		ASN			-1.390	90.525	43.857		32.69	A	N
50	MOTA	1866 1867	C	ASN ASN			-0.526 -1.389	88.926 88.928	45.965 46.843		28.67 29.64	A A	C
50	ATOM	1868	N	PRO			0.562	89.706	46.044		29.84	A.	N
	ATOM	1869	CD	PRO			1.612	89.829	45.019		28.83	A	c
	MOTA	1870	CA	PRO			0.832	90.611	47.172	1.00	31.07	A	c
	ATOM	1871	CB	PRO			2.013	91.437	46.675	1.00	30.37	A	C
55		1872	CG	PRO			2.734	90.479	45.790		30.85	A	C
	MOTA	1873	C	PRO			-0.328	91.496	47.624		32.07	A.	C
	MOTA	1874	0	PRO			-0.483	91.754	48.820	1.00	32.30	A	0
	ATOM	1875	N	SER			-1.131	91.966	46.671	1.00	32.61	A	N C
60	ATOM ATOM	1876 1877	CB	SER			-2.261 -2.760	92.834 93.547	46.987 45.720	1.00	35.81	A A	c
00	ATOM	1878	OG	SER	2	368	-3.206	92.623	44.736	1.00	36.05	A.	o
	ATOM	1879	c	SER			-3.413	92.088	47.656	1.00	35.02	A.	c
	ATOM	1880	ō	SER			-4.290	92.706	48.258	1.00	37.52	A	ŏ
	ATOM	1881	N	GLN	Α	369	-3.418	90.763	47.554	1.00	34.24	A	N
65		1882	CA	GLN			-4.475	89.975	48.176	1.00	33.87	A.	С
	ATOM	1883	CB	GLN			-4.644	88.637	47.463		36.07	A	С
	ATOM	1884	CG	GLN			-5.499	88.695	46.218		40.88	A	C
	ATOM	1885	CD	GLN			-5.478	87.382	45.463		44.11	A.	C
70	ATOM	1886 1887	OE1	GLN			-5.619 -5.303	86.308 87.457	46.059 44.145		45.39 45.10	A A	N
, 0	ATOM	1888	C	GLN			-4.214	89.721	49.653		32.42	A A	C
	ATOM	1889	ŏ	GLN			-5.045	89.136	50.336		31.67	A	ō

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	ATOM	1890	N	ARG	Α	370	-3.053	90.149	50.141		31.86		A	N
	ATOM	1891	CA			370	-2.714	89.968	51.549		30.59	- 4		C
	ATOM	1892	CB	ARG			-1.193	89.979	51.741		27.86	1		C
5	ATOM	1893 1894	CD	ARG			-0.498 1.015	88.834 89.020	51.047 50.987		27.06	1		C
,	ATOM	1895	NE	ARG			1.552	88.214	49.901		23.24	- 2		N
	ATOM	1896	CZ	ARG			2.744	88.385	49.344		22.14	- 3		c
	ATOM	1897		ARG			3.557	89.340	49.777		19.46			N
	MOTA	1898				370	3.098	87.618	48.314		20.24			N
10	ATOM	1899 1900	C	ARG			-3.349 -3.380	91.103 92.244	52.344 51.887		30.03	1		C
	ATOM	1901	N				-3.861	90.801	53.549		29.42	- 2		N
	ATOM	1902	CD		A	371	-3.861	89.468	54.180		28.61	- 3		Ĉ
	ATOM	1903	CA	PRO	А	371	-4.506	91.783	54.426		29.38		A.	С
15	ATOM	1904	CB		Α	371	-5.105	90.911	55.524		28.93	1		C
	ATOM	1905	CG	PRO		371	-4.130 -3.579	89.800	55.626 54.995	1.00	27.39	- 1		C
	ATOM	1906 1907	0		A	371 371	-2.356	92.856 92.719	54.979	1.00	30.07	2		ò
	ATOM	1908	N		Ã		-4.179	93.932	55.489	1.00		- 3		N
20	ATOM	1909	CA	MET	A	372	-3.422	95.014	56.095	1.00	28.79		A	С
	MOTA	1910	CB	MET	Α	372	-4.297	96.255	56.209	1.00	32.05	1		C
	ATOM	1911	CG	MET	A		-4.983	96.641	54.909	1.00		1		C
	MOTA	1912 1913	SD	MET	A	372 372	-6.339 -5.396	97.820 99.295	55.165 55.623		45.86	1		S
25	ATOM	1914	CE	MET		372	-3.050	94.511	57.484		27.02	- 3		č
	ATOM	1915	ŏ	MET		372	-3.635	93.542	57.965		25.83	- 3		ŏ
	MOTA	1916	N	LEU		373	-2.084	95.160	58.126		26.03			N
	MOTA	1917	CA	LEU		373	-1.650	94.759	59.462		24.32	- 4		С
30	ATOM ATOM	1918 1919	CB	LEU		373 373	-0.422 0.874	95.570 95.259	59.886 59.134		24.26	1		C
50	ATOM	1920	CD1			373	1.971	96.239	59.545		22.42	- 1		č
	ATOM	1921	CD2			373	1.291	93.821	59.422		22.22	- 3		č
	MOTA	1922	C	LEU			-2.756	94.910	60.504		23.93			С
0.5	MOTA	1923	0	LEU			-2.789	94.181	61.488		24.38	- 4		0
35	MOTA MOTA	1924 1925	N CA	ALA ALA			-3.666 -4.772	95.852 96.080	60.281 61.203		24.38	1		N
	ATOM	1926	CB	ALA			-5.503	97.370	60.836		26.79	- 1		ċ
	ATOM	1927	c	ALA			-5.741	94.911	61.164		23.14	- 3		č
	MOTA	1928	0	ALA	А	374	-6.432	94.637	62.150		22.46			0
40	MOTA	1929	N	GLU			-5.798	94.227	60.022		23.02			N
	MOTA	1930 1931	CA	GLU			-6.694 -6.908	93.084 92.745	59.875 58.398		25.10	1		C
	ATOM	1932	CG	GLU			-7.552	93.858	57.593	1.00				č
	ATOM	1933	CD	GLU			-7.814	93.459	56.151	1.00	30.04	- 3		č
45	MOTA	1934	OE1	GLU			-8.843	92.800	55.883		33.09			0
	ATOM	1935	OE2	GLU			-6.984	93.796	55.289		29.56	- 1		0
	MOTA	1936 1937	C	GLU			-6.143 -6.910	91.864 91.011	60.612 61.063		25.25 27.99			C
	ATOM	1938	N	VAL			-4.820	91.785	60.727		22.91			N
50	ATOM	1939	CA	VAL			-4.175	90.687	61.439	1.00	21.50		١.	C
	ATOM	1940	CB	VAL		376	-2.643	90.662	61.187	1.00	21.90	1		С
	ATOM	1941		VAL			-1.976	89.654	62.125		19.51	- 1		C
	ATOM	1942 1943	CG2	VAL		376	-2.355 -4.405	90.313 90.862	59.729 62.944	1.00	22.63 21.43	- 1		C
55	ATOM	1944	ò	VAL			-4.725	89.906	63.653		19.70			ŏ
	ATOM	1945	N	LEU			-4.241	92.090	63.422	1.00	19.23	- 3		N
	ATOM	1946	CA	LEU			-4.426	92.375	64.837		22.49		A	С
	ATOM	1947	CB	LEU			~4.002	93.815	65.142 64.962	1.00	22.58			C
60	ATOM	1948 1949	CG CD1	LEU		377 377	-2.498 -2.172	94.047 95.525	64.951		22.54	1	a A	c
00	ATOM	1950				377	-1.753	93.341	66.092		22.08			c
	ATOM	1951	C	LEU	А	377	-5.869	92.143	65.269	1.00	25.05		A.	C
	ATOM	1952	0	LEU		377	-6.141	91.905	66.443		26.04	4		0
65	ATOM	1953	N	GLU			-6.787	92.177	64.308		24.26			N
υɔ	ATOM	1954 1955	CB		A A	378 378	-8.193 -9.032	91.983 93.046	64.611 63.890		25.18 27.95			C
	ATOM	1956	CG	GLU		378	-8.848	94.444	64.452		31.63		ì	c
	ATOM	1957	CD	GLU	Α	378	-9.693	95.484	63.743	1.00	33.54		A	С
	ATOM	1958	OE1	GLU			-9.894	96.568	64.334		35.00	- 4		0
70		1959	OE2	GLU			-10.147	95.220	62.605		31.59		A.	0
	ATOM ATOM	1960 1961	C	GLU			-8.713 -9.883	90.597 90.301	64.251 64.473		24.15		ž.	C
	AT OF	1501	0	310	^	3,0	-3.663	20.301	J4.4/3	1.00	21.00		-	_

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	ATOM	1962	N	HIS	A	379	-7.860	89.742	63.702	1.00	22.41	A	N
	ATOM	1963	CA	HIS		379	-8.322	88.410	63.337		22.38	A	C
	ATOM	1964	CB	HIS		379	-7.200	87.624	62.665		18.92	A	C
5	ATOM	1965 1966	CG CD2	HIS		379 379	-7.650 -7.936	86.333 86.009	62.050 60.767	1.00	16.62 15.24	A. A.	C
э	ATOM	1966		HIS		379	-7.834	85.181	62.786	1.00	15.11	A.	N
	ATOM	1968		HIS		379	-8.208	84.202	61.982	1.00	16.55	A	C
	ATOM	1969		HIS	Α	379	-8.278	84.678	60.751	1.00	17.07	A.	N
	ATOM	1970	C	HIS		379	-8.818	87.695	64.595	1.00	22.89	A	C
10	ATOM	1971	0	HIS		379	-8.211	87.802	65.659	1.00	24.73	A	0
	ATOM	1972 1973	CD N	PRO		380 380	-9.948 -10.751	86.978 86.800	64.489 63.266	1.00	22.77	A. A	C
	ATOM	1974	CA	PRO		380	-10.544	86.247	65.614	1.00	22.16	A	č
	MOTA	1975	CB	PRO		380	-11.777	85.580	64.984	1.00	22.20	A	С
15	MOTA	1976	CG	PRO			-11.422	85.482	63.529	1.00	24.64	A	С
	MOTA	1977	С	PRO			-9.633	85.256	66.351	1.00	21.00	A	C
	MOTA	1978	0	PRO			-9.762	85.078 84.613	67.563 65.627	1.00	19.68	A. A.	N O
	ATOM	1979 1980	N CA	TRP			-8.722 -7.801	83.666	66.246	1.00	18.47	a. A	C
20	ATOM	1981	CB	TRP			-7.098	82.827	65.172	1.00	17.30	Ā	č
	ATOM	1982	CG	TRP			-6.164	81.805	65.737	1.00	19.05	A	C
	ATOM	1983	CD2	TRP			-4.733	81.895	65.800	1.00	18.83	A.	С
	ATOM	1984	CE2			381	-4.270	80.732	66.456	1.00	19.95	A. A.	C
25	ATOM	1985 1986	CE3	TRP			-3.800 -6.499	82.846 80.628	65.366 66.336	1.00	19.48 18.42	A.	c
23	ATOM	1986	NE1	TRP			-5.368	79.975	66.771	1.00	18.35	A.	N
	ATOM	1988	CZ2	TRP			-2.907	80.493	66.690	1.00	18.02	A	С
	ATOM	1989	CZ3			381	-2.440	82.609	65.597	1.00	19.48	A	С
	MOTA	1990	CH2	TRP		381	-2.011	81.439	66.254	1.00	19.82	A.	c
30	ATOM	1991	c	TRP			-6.764	84.430	67.088 68.176	1.00	18.12	A A	C
	ATOM ATOM	1992 1993	N O	TRP		381	-6.385 -6.324	83.991 85.579	66.587	1.00	18.20	a A	N
	ATOM	1994	CA			382	-5.347	86.410	67.296		19.68	A.	c
	ATOM	1995	CB			382	-4.875	87.569	66.394	1.00	17.49	A	C
35	ATOM	1996	CG2	ILE		382	-4.118	88.599	67.213	1.00	20.81	A	C
	ATOM	1997	CG1	ILE		382	-4.020	87.021	65.243		18.99	A	C
	ATOM	1998 1999	CD1			382 382	-2.653 -5.932	86.493 86.997	65.655 68.592	1.00		A A	c
	ATOM	2000	ŏ	ILE			-5.271	87.019	69.642	1.00	21.36	Ā	ŏ
40	ATOM	2001	N	THR			-7.174	87.469	68.504	1.00	21.35	A	N
	ATOM	2002	CA	THR			-7.886	88.068	69.632		22.03	A	C
	ATOM	2003	CB	THR			-9.213	88.734	69.143		24.29	A A	C
	ATOM	2004	OG1 CG2	THR			-8.912 -10.140	89.957 89.028	68.457 70.312		28.50 28.56	A A	c
45	ATOM ATOM	2005	CGZ	THR			-8.225	87.040	70.713		21.21	Ä	č
45	ATOM	2007	ŏ	THR			-8.139	87.316	71.904	1.00	19.20	A	0
	ATOM	2008	N	ALA	Α	384	-8.622	85.849	70.285	1.00	21.12	A	N
	ATOM	2009	CA	ALA			-8.986	84.788	71.217		19.34	A	C
50	ATOM	2010	CB	ALA			-9.661 -7.822	83.649 84.231	70.448		16.55 21.30	A A	C
30	ATOM ATOM	2011	0	ALA			-7.980	83.995	73.259		22.43	Ã.	ŏ
	ATOM	2013	N	ASN			-6.661	84.040	71.416	1.00	20.05	A	N
	ATOM	2014	CA	ASN	Α	385	-5.503	83.449	72.091	1.00	22.78	A	C
	MOTA	2015	CB	ASN			-4.883	82.377	71.195		20.49	A A	C
55	ATOM	2016	CG	ASN			-5.871	81.286 80.569	70.817 71.674		21.65	A A	C
	ATOM ATOM	2017 2018	OD1 ND2				-6.380 -6.148	81.160	69.525		19.14	A	N
	ATOM	2019	C	ASN			-4.385	84.356	72.593		25.16	A	c
	ATOM	2020	ŏ	ASN			-3.472	83.883	73.267	1.00	27.83	A	0
60	ATOM	2021	N			386	-4.426	85.642	72.274		26.88	A	N
	ATOM	2022	CA			386	-3.375	86.536	72.739		29.74	A A	C
	ATOM	2023	CB			386 386	-3.385 -2.391	87.834 88.717	71.940		30.28	A A	C
	ATOM	2024	C			386	-3.559	86.851	74.218		32.93	A	č
65	ATOM	2026	õ			386	-4.677	87.088	74.676	1.00	32.42	A	0
	MOTA	2027	M	SER	A	387	-2.461	86.844	74.967	1.00	34.64	A	N
	MOTA	2028	CA	SER		387	-2.524	87.144	76.393		37.99	A	C
	MOTA	2029	CB	SER		387	-1.376	86.454 86.876	77.141 76.662	1.00	38.92 37.92	A A	C
70	MOTA MOTA	2030	OG C	SER		387 387	-0.112 -2.451	88.652	76.599		39.48	A	c
,0	ATOM	2032	õ			387	-2.459	89.135	77.728		40.65	A	0
	ATOM	2033	N			388	-2.387	89.383	75.489		41.58	A	N

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	ATOM	2034	CA		A 388	-2.320	90.844	75.487	1.00 43.93	A	C
	ATOM	2035	CB		A 388	-3.340	91.441	76.466	1.00 43.62	A	С
	ATOM	2036	CD		A 388 A 388	-4.758 -5.787	90.887 91.767	76.316 77.016	1.00 43.37 1.00 43.10	A A	C
5	ATOM	2037	CE		A 388	-6.533	92.633	75.989	1.00 43.10	A	c
-	ATOM	2039	NZ		A 388	-5.609	93.345	75.045	1.00 42.84	A	N
	ATOM	2040	C		A 388	-0.918	91.354	75.822	1.00 45.61	A	C
	ATOM	2041	0	LYS	A 388	-0.649	91.581	77.023	1.00 46.51	A	0
	ATOM	2042	OXT	LYS	A 388	-0.100	91.503	74.881	1.00 46.24	A	0
10	TER	2043			A 388					_	_
	ATOM	2044	CB		B 126 B 126	10.213 11.292	7.246	17.228 16.169	1.00 52.35 1.00 53.31	B B	C
	ATOM	2046	CD		B 126	12.534	6.382	16.706	1.00 54.51	В	c
	ATOM	2047	OE1		B 126	13.488	6.131	15.966	1.00 55.84	В	ŏ
15	MOTA	2048	NE2	GLN	B 126	12.526	6.065	17.999	1.00 53.41	В	N
	MOTA	2049	С		B 126	8.987	9.170	16.193	1.00 50.24	В	C
	MOTA	2050	0		B 126	8.930	9.438	14.994	1.00 50.75	В	0
	ATOM ATOM	2051 2052	N CA		B 126 B 126	8.388 8.864	6.816 7.730	15.605 16.685	1.00 51.32 1.00 51.36	B B	N
20	ATOM	2052	N		B 127	9.168	10.087	17.137	1.00 48.65	В	N
	ATOM	2054	CA		B 127	9.279	11.516	16.855	1.00 45.05	В	c
	ATOM	2055	CB		B 127	9.752	12.240	18.112	1.00 45.82	В	Ċ
	ATOM	2056	CG		B 127	8.716	12.256	19.197	1.00 48.91	В	С
o.e	ATOM	2057	CD2		B 127	7.325	12.583	19.052	1.00 49.46	В	C
25	ATOM	2058 2059	CE2 CE3		B 127 B 127	6.741 6.517	12.502 12.937	20.336 17.962	1.00 50.15	B B	C
	ATOM	2059	CD1		B 127	8.911	11.997	20.523	1.00 50.60	B	C
	ATOM	2061			B 127	7.730	12.143	21.214	1.00 50.57	В	N
	ATOM	2062	CZ2		B 127	5.384	12.764	20.563	1.00 51.76	В	C
30	ATOM	2063	CZ3		B 127	5.163	13.197	18.186	1.00 51.62	В	С
	ATOM	2064	CH2		B 127	4.613	13.108	19.479	1.00 51.32	В	C
	ATOM ATOM	2065 2066	0		B 127 B 127	10.131 11.322	11.952 11.660	15.671 15.593	1.00 42.62 1.00 42.25	B B	C
	ATOM	2067	N		B 128	9.488	12.664	14.749	1.00 39.75	B	N
35	ATOM	2068	CA		B 128	10.141	13.206	13.564	1.00 36.83	В	c
	ATOM	2069	CB		B 128	9.858	12.342	12.342	1.00 37.27	В	C
	ATOM	2070	C		B 128	9.533	14.584	13.386	1.00 33.84	В	C
	ATOM	2071	0		B 128	8.469	14.862	13.929	1.00 33.46	В	0
40	ATOM	2072	N CA		B 129 B 129	10.201 9.718	15.443 16.798	12.630 12.419	1.00 32.37 1.00 32.04	B B	C
70	ATOM	2074	CB		B 129	10.708	17.570	11.548	1.00 31.51	В	c
	ATOM	2075	CG		B 129	10.548	19.091	11.537	1.00 33.77	В	C
	ATOM	2076	CD1		B 129	10.560	19.625	12.968	1.00 33.40	В	С
	ATOM	2077	CD2		B 129	11.673	19.708	10.731	1.00 32.31	В	C
45	ATOM	2078 2079	C		B 129 B 129	8.321 7.479	16.854 17.645	11.796 12.226	1.00 31.97 1.00 31.99	B B	C
	ATOM	2079	N		B 130	8.082	16.007	10.797	1.00 31.39	В	N
	ATOM	2081	CA		B 130	6.803	15.951	10.091	1.00 31.88	В	č
	ATOM	2082	CB		B 130	6.866	14.898	8.983	1.00 31.86	В	C
50		2083	C		B 130	5.609	15.677	10.995	1.00 31.10	В	C
	ATOM	2084	0	ALA		4.465	15.794	10.568	1.00 32.53	В	0
	ATOM ATOM	2085 2086	N CA		B 131 B 131	5.871 4.800	15.312 15.038	12.243 13.193	1.00 30.37 1.00 30.59	B B	C
	ATOM	2087	CB		B 131	5.329	14.156	14.328	1.00 30.33	В	č
55	ATOM	2088	CG		B 131	5.607	12.727	13.884	1.00 36.29	В	č
	ATOM	2089	OD1		B 131	6.370	12.025	14.582	1.00 36.01	В	0
	ATOM	2090	OD2		B 131	5.053	12.302	12.847	1.00 36.71	В	0
	ATOM	2091	C		B 131 B 131	4.197	16.309	13.796	1.00 29.73	В	C
60	ATOM	2092 2093	N		B 132	3.185 4.800	16.242 17.462	14.492 13.512	1.00 30.13 1.00 28.26	B B	O N
00	ATOM	2094	CA	PHE		4.344	18.725	14.092	1.00 25.47	В	C
	ATOM	2095	CB		B 132	5.417	19.272	15.039	1.00 25.53	B	č
	ATOM	2096	CG		B 132	5.944	18.268	16.020	1.00 25.89	В	С
c =	ATOM	2097	CD1	PHE		5.301	18.056	17.234	1.00 27.37	В	C
65	MOTA	2098	CD2 CE1		B 132 B 132	7.087	17.536	15.732	1.00 26.04	В	C
	ATOM ATOM	2099 2100	CE1	PHE		5.791 7.584	17.130 16.608	18.144	1.00 28.04 1.00 26.31	B B	c
	ATOM	2101	CZ		B 132	6.937	16.403	17.839	1.00 20.51	В	c
	ATOM	2102	C	PHE	B 132	4.020	19.855	13.127	1.00 25.28	В	C
70	ATOM	2103	0	PHE		4.581	19.946	12.039	1.00 23.06	В	0
	ATOM	2104	N	GLU		3.113	20.724	13.567	1.00 24.47	В	N
	MOTA	2105	CA	GTO	В 133	2.751	21.929	12.835	1.00 24.02	В	C

							-74-				
	ATOM	2106	СВ		В 133	1.234	22.125	12.779	1.00 26.65	В	С
	ATOM	2107	CG		B 133	0.586	21.444	11.597	1.00 32.34	В	C
	ATOM	2108	CD	GLU :	в 133	-0.806	21.962	11.312	1.00 36.67	В	C
5	ATOM	2109 2110	OE1			-1.355	21.615	10.245	1.00 38.29	В	0
,	ATOM	2111	C		B 133	-1.348 3.387	22.715 23.029	12.151 13.678	1.00 38.65	B B	0
	ATOM	2112	ō	GLU :	B 133	3.123	23.122	14.873	1.00 22.07	В	C
	ATOM	2113	N	ILE :		4.228	23.842	13.051	1.00 22.05	В	N
	MOTA	2114	CA		B 134	4.957	24.924	13.718	1.00 20.74	В	c
10	ATOM	2115	CB	ILE :	B 134	6.356	25.077	13.065	1.00 22.02	B	č
	ATOM	2116	CG2	ILE I		7.127	26.232	13.692	1.00 19.99	В	C
	ATOM	2117 2118	CG1	ILE I		7.121	23.758	13.219	1.00 22.38	В	C
	ATOM	2119	CD1	ILE I		8.451 4.226	23.728 26.259	12.488	1.00 26.58	B	С
15	ATOM	2120	ŏ	ILE I		3.688	26.259	12.618	1.00 20.52 1.00 21.50	В	C
	ATOM	2121	N	GLY I		4.222	26.989	14.778	1.00 19.55	В	N
	ATOM	2122	CA	GLY I		3.547	28.282	14.846	1.00 19.33	В	c
	ATOM	2123	С	GLY 1		4.485	29.464	15.035	1.00 19.91	В	č
	ATOM	2124	0		3 135	5.614	29.435	14.563	1.00 18.49	В	0
20	ATOM	2125	N		3 136	4.034	30.499	15.739	1.00 21.61	В	N
	MOTA MOTA	2126 2127	CA	ARG I		4.857 4.014	31.695 32.824	15.970	1.00 23.20	В	C
	ATOM	2128	CG		3 136	3.656	32.619	16.570 18.042	1.00 24.31 1.00 27.58	B B	c
	ATOM	2129	CD		3 136	2.652	33.652	18.548	1.00 28.19	В	č
25	ATOM	2130	NE	ARG I		2.162	33.295	19.877	1.00 29.58	В	N
	ATOM	2131	cz		3 136	2.671	33.747	21.023	1.00 30.89	В	c
	ATOM	2132	NH1	ARG I		3.692	34.598	21.016	1.00 28.09	В	N
	ATOM	2133	NH2	ARG I		2.167	33.326	22.182	1.00 29.68	В	N
30	ATOM	2134 2135	C	ARG I		6.049 6.019	31.460 30.597	16.895 17.762	1.00 22.61	В	C
50	ATOM	2136	N	PRO I		7.126	32.231	16.709	1.00 22.20 1.00 24.01	В	O N
	ATOM	2137	CD		3 137	7.425	33.170	15.611	1.00 24.72	В	C
	ATOM	2138	CA	PRO I		8.287	32.047	17.581	1.00 23.55	В	č
2.5	ATOM	2139	CB	PRO I		9.393	32.798	16.840	1.00 26.09	В	С
35	MOTA MOTA	2140 2141	CG		3 137	8.637	33.905	16.144	1.00 26.11	В	C
	ATOM	2142	C		3 137 3 137	7.976 7.350	32.627 33.682	18.965 19.088	1.00 23.34	В	C
	ATOM	2143	N	LEU		8.390	31.909	20.000	1.00 22.43	B B	N
	ATOM	2144	CA	LEU I		8.153	32.316	21.383	1.00 25.08	В	Č
40	ATOM	2145	CB	LEU I		7.909	31.077	22.247	1.00 23.93	В	С
	ATOM	2146	CG	PEA B		6.501	30.564	22.574	1.00 25.09	В	C
	ATOM	2147 2148	CD1 CD2	LEU I		5.475 6.575	30.991	21.532	1.00 21.71	В	C
	ATOM	2149	C	LEU I		9.361	29.054 33.076	22.715 21.908	1.00 22.09 1.00 27.37	B B	C
45	ATOM	2150	ŏ	LEU I		9.253	33.860	22.842	1.00 27.37	В	0
	ATOM	2151	N	GLY I		10.511	32.831	21.292	1.00 30.52	В	N
	ATOM	2152	CA	GLY I		11.736	33.487	21.701	1.00 33.40	В	C
	ATOM	2153	C	GLY I		12.887	33.087	20.796	1.00 36.61	В	C
50	MOTA	2154 2155	O N	GLY E		12.829	32.049	20.125	1.00 34.75	В	0
50	ATOM	2156	CA	ALA I		13.931 15.111	33.917 33.669	20.775 19.952	1.00 38.80 1.00 41.45	B B	N
	ATOM	2157	CB	ALA E		15.197	34.703	18.839	1.00 41.02	В	č
	MOTA	2158	C	ALA E		16.348	33.742	20.833	1.00 42.68	В	č
	MOTA	2159	0	ALA E		16.614	34.774	21.443	1.00 44.14	В	0
55	ATOM	2160	N	ALA E		17.091	32.640	20.905	1.00 43.65	В	N
	ATOM	2161 2162	CA	ALA E		18.295	32.567	21.728	1.00 43.81	В	C
	ATOM	2163	C	ALA E		18.233 19.553	31.342 32.515	22.638	1.00 45.73	В	C
	ATOM	2164	ŏ	ALA E		19.501	32.748	19.669	1.00 43.24	В	0
60	ATOM	2165	N	ALA E		20.682	32.203	21.502	1.00 43.17	В	N
	ATOM	2166	CA	ALA E		21.956	32.136	20.794	1.00 43.89	В	c
	ATOM	2167	CB	ALA I		23.107	32.336	21.774	1.00 43.83	В	C
	ATOM ATOM	2168 2169	C	ALA E		22.146	30.826	20.032	1.00 44.12	В	C
65	ATOM	2170	N	PHE E		22.701 21.682	30.817 29.723	18.932 20.612	1.00 45.04 1.00 43.15	В	0
00	ATOM	2171	CA	PHE E		21.829	28.421	19.973	1.00 43.15	В	N
	ATOM	2172	CB	PHE E	143	22.102	27.350	21.025	1.00 43.72	В	č
	MOTA	2173	CG	PHE E		23.254	27.671	21.931	1.00 47.41	В	C
70	MOTA	2174	CD1	PHE E		23.098	28.563	22.986	1.00 48.28	В	C
/0	ATOM	2175 2176	CD2 CE1	PHE E		24.496	27.079	21.733	1.00 47.70	В	С
	ATOM	2177		PHE E		24.162 25.564	28.858 27.368	23.832 22.572	1.00 49.52 1.00 48.56	В	C
					45	25.564	21.300	44.574	1.00 48.56	В	C

							-75-				
	MOTA	2178	CZ	PHE	B 143	25.398	28.259	23.624	1.00 48.11	В	С
	MOTA	2179	С		B 143	20.625	28.002	19.127	1.00 39.85	В	č
	ATOM	2180	0	PHE		20.673	26.972	18.453	1.00 37.97	В	0
5	MOTA	2181	N		B 144	19.554	28.792	19.164	1.00 37.20	В	N
,	ATOM	2182 2183	CA		B 144 B 144	18.374	28.461	18.386	1.00 35.94	В	C
	ATOM	2184	0		B 144	17.111 17.172	29.160 30.161	18.851	1.00 35.06	В	С
	ATOM	2185	N		B 145	15.959	28.628	19.565 18.449	1.00 34.22 1.00 33.13	B	0
	ATOM	2186	CA		B 145	14.682	29.228	18.826	1.00 33.13	В	N
10	ATOM	2187	CB	ASN		14.082	29.980	17.639	1.00 33.45	В	č
	ATOM	2188	CG	ASN	B 145	15.124	30.694	16.824	1.00 36.83	В	č
	ATOM	2189		ASN		15.849	30.072	16.051	1.00 39.85	В	ō
	ATOM	2190	ND2			15.220	32.010	16.999	1.00 39.53	В	N
15	MOTA	2191	c		B 145	13.654	28.225	19.318	1.00 27.19	В	С
13	MOTA	2192 2193	N O		B 145 B 146	13.751	27.026	19.053	1.00 26.12	В	0
	ATOM	2193	CA		B 146	12.663 11.568	28.745 27.951	20.030	1.00 23.46	В	N
	ATOM	2195	CB	VAL		11.382	28.182	20.568	1.00 21.53 1.00 21.61	B B	C
	ATOM	2196			B 146	10.329	27.242	22.623	1.00 21.81	В	c
20		2197	CG2		B 146	12.688	27.990	22.807	1.00 26.97	В	č
	ATOM	2198	C	VAL	B 146	10.307	28.447	19.865	1.00 20.89	В	č
	ATOM	2199	0		B 146	10.087	29.657	19.774	1.00 18.61	В	ŏ
	ATOM	2200	N		B 147	9.489	27.518	19.379	1.00 18.85	В	N
25	ATOM ATOM	2201	CA		B 147	8.254	27.866	18.688	1.00 18.39	В	C
23	ATOM	2202 2203	CB		B 147 B 147	8.273 9.420	27.362	17.239	1.00 17.65	В	. с
	ATOM	2204	CD1			10.654	27.846 27.186	16.400 16.409	1.00 17.80	В	C
	ATOM	2205	CE1	TYR		11.726	27.653	15.629	1.00 19.71 1.00 20.17	B B	C
	ATOM	2206	CD2	TYR		9.281	28.976	15.598	1.00 20.17	В	c
30	ATOM	2207	CE2	TYR		10.336	29.447	14.823	1.00 16.88	В	č
	ATOM	2208	CZ	TYR		11.550	28.791	14.840	1.00 17.99	В	č
	ATOM	2209	OH	TYR		12.582	29.292	14.078	1.00 21.66	В	ō
	MOTA	2210	C	TYR		7.050	27.218	19.349	1.00 17.88	В	C
35	MOTA	2211 2212	O N	TYR LEU	B 147	7.180	26.186	20.000	1.00 17.17	В	0
33	ATOM	2212	CA	LEU :		5.880 4.661	27.829	19.188	1.00 17.80	В	N
	ATOM	2214	CB	LEU :		3.478	27.208 28.172	19.688 19.616	1.00 18.36 1.00 22.50	B B	C
	ATOM	2215	CG	LEU	B 148	2.102	27.595	19.990	1.00 23.22	В	c
	ATOM	2216		LEU :		2.017	27.353	21.494	1.00 24.62	В	c
40	MOTA	2217	CD2	PER :		1.016	28.563	19.559	1.00 25.28	В	č
	MOTA	2218	С	LEU :		4.475	26.107	18.641	1.00 19.19	В	c
	MOTA	2219	0	LEU :		4.849	26.289	17.476	1.00 18.41	В	0
	ATOM	2220 2221	N CA	ALA I		3.941	24.959	19.034	1.00 18.74	В	N
45	ATOM	2222	CB	ALA :		3.734 5.005	23.900 23.057	18.063 17.907	1.00 21.02	В	С
	ATOM	2223	c	ALA I		2.560	23.018	18.429	1.00 22.54 1.00 22.53	B	C
	ATOM	2224	ō	ALA I		2.109	23.002	19.573	1.00 22.04	В	ŏ
	MOTA	2225	N		B 150	2.060	22.286	17.444	1.00 23.48	В	N
	MOTA	2226	CA		B 150	0.932	21.402	17.667	1.00 26.45	В	Ĉ
50	MOTA	2227	CB		B 150	-0.349	22.081	17.176	1.00 27.56	В	C
	ATOM ATOM	2228	CD		B 150 B 150	-1.626	21.299	17.419	1.00 31.39	В	C
	ATOM	2230	NE		B 150	-2.817 -2.772	22.249 23.313	17.534 16.534	1.00 33.89 1.00 37.25	В	C
	ATOM	2231	CZ		B 150	-3.463	24.447	16.616	1.00 37.25	B	N
55	ATOM	2232		ARG I		-4.258	24.669	17.655	1.00 39.33	В	N
	ATOM	2233		ARG I		-3.350	25.367	15.664	1.00 37.88	В	N
	MOTA	2234	C		B 150	1.157	20.075	16.957	1.00 27.39	в	č
	MOTA	2235	0		B 150	1.540	20.044	15.785	1.00 26.15	В	ō
60	MOTA	2236	N		B 151	0.953	18.978	17.680	1.00 28.95	В	N
00	ATOM	2237 2238	CB	GLU I		1.130	17.657	17.092	1.00 33.02	В	C
	ATOM	2239	CG	GLU I		1.153	16.597 15.344	18.186 17.795	1.00 34.21 1.00 39.51	В	С
	MOTA	2240	CD	GLU I		1.687	14.213	18.781	1.00 43.41	B B	C
	MOTA	2241		GLU I		1.948	14.412	19.991	1.00 44.45	В	0
65	ATOM	2242	OE2	GLU I	3 151	1.257	13.122	18.342	1.00 46.66	В	ö
	MOTA	2243	C	GLU E		-0.031	17.402	16.123	1.00 33.90	В	č
	ATOM	2244	0	GLU I		-1.187	17.611	16.470	1.00 31.69	В	0
	ATOM	2245		LYS I		0.281	16.958	14.911	1.00 36.17	В	N
70	ATOM	2246 2247	CB	LYS E	3 152 3 152	-0.747	16.718	13.901	1.00 39.16	В	С
,,,	ATOM	2248		LYS I		-0.103 0.598	16.292 17.422	12.579 11.855	1.00 38.11	В	c
	MOTA	2249		LYS I		1.208	16.952	10.554	1.00 37.99 1.00 39.08	B	C

							-76-				
	ATOM	2250	CE	LYS B	152	1.924	18.091	9.855	1.00 40.02	В	C
	ATOM	2251	NZ	LYS B		2.654	17.635	8.642	1.00 41.02	В	N
	MOTA	2252	С	LYS E		-1.845	15.725	14.270	1.00 41.64	B	C
5	MOTA	2253	O N	LYS E		-3.033 -1.459	16.047 14.523	14.171 14.688	1.00 44.21	В	N
Э	ATOM	2254 2255	CA	GLN E		-2.445	13.505	15.040	1.00 46.53	В	c
	ATOM	2256	CB	GLN E		-1.756	12.244	15.553	1.00 48.92	В	C
	ATOM	2257	CG	GLN E		-2.672	11.035	15.561	1.00 53.13	В	C
	ATOM	2258	CD	GLN E		-3.378	10.842	14.226	1.00 55.60	В	c
10	ATOM	2259	OE1	GLN E		-2.735	10.731	13.177	1.00 56.44 1.00 55.73	B	O N
	MOTA	2260	NE2	GLN E		-4.708 -3.427	10.807	14.260 16.082	1.00 55.73	В	C
	MOTA	2261 2262	C	GLN E		-4.626	14.116	15.825	1.00 47.04	В	ő
	ATOM	2263	N	SER I		-2.926	14.344	17.265	1.00 46.37	В	N
15	ATOM	2264	CA	SER I		-3.791	14.879	18.305	1.00 46.19	В	C
	ATOM	2265	CB	SER I		-3.206	14.591	19.690	1.00 45.90	В	C
	ATOM	2266	OG	SER I		-1.871	15.057	19.798	1.00 45.56 1.00 46.16	B B	0
	ATOM	2267	C	SER I		-3.847 -3.415	16.379 16.846	18.046 16.995	1.00 45.16	В	0
20	MOTA	2268 2269	O N	SER I	3 154	-4.387	17.139	18.981	1.00 45.67	В	N
20	ATOM	2270	CA		3 155	-4.450	18.582	18.806	1.00 45.70	В	С
	ATOM	2271	CB	LYS I		-5.916	19.031	18.799	1.00 48.89	В	C
	ATOM	2272	CG	LYS I		-6.128	20.540	18.761	1.00 52.40	В	C
	ATOM	2273	CD	LYS I		-6.349	21.108	20.159	1.00 53.23	B	C
25	ATOM	2274	CE	LYS I		-6.084 -4.697	22.601	20.182 19.726	1.00 54.16 1.00 53.54	В	N
	ATOM	2275 2276	NZ C	LYS I		-4.697	19.222	19.959	1.00 42.90	В	c
	ATOM	2277	0	LYS	a 155	-3.770	20.423	20.207	1.00 43.52	В	ō
	ATOM	2278	N	PHE I	156	-2.892	18.397	20.644	1.00 39.07	В	N
30	ATOM	2279	CA	PHE I	B 156	-2.108	18.824	21.796	1.00 35.93	В	C
	ATOM	2280	CB		B 156	-1.375	17.615	22.377	1.00 37.42	В	C
	ATOM	2281	CG		В 156	-0.841	17.834 18.157	23.761 24.806	1.00 39.54	B B	C
	ATOM	2282 2283		PHE I		-1.699 0.521	17.705	24.024	1.00 40.10	В	č
35	ATOM	2284		PHE		-1.209	18.351	26.099	1.00 40.25	В	C
55	ATOM	2285	CE2			1.024	17.897	25.316	1.00 40.40	В	C
	ATOM	2286	CZ		В 156	0.156	18.220	26.354	1.00 40.47	В	C
	ATOM	2287	C		B 156	-1.111	19.943	21.487	1.00 32.41	B B	C
	ATOM	2288	0	PHE		-0.328 -1.153	19.846 20.999	20.544	1.00 31.99 1.00 28.30	В	N
40	MOTA	2289 2290	N CA	ILE	B 157 B 157	-0.270	22.153	22.146	1.00 27.01	В	c
	ATOM	2291	CB		B 157	-0.933	23.445	22.684	1.00 28.09	В	C
	ATOM	2292		ILE		0.042	24.608	22.590	1.00 29.72	В	С
	ATOM	2293	CG1		в 157	-2.212	23.754	21.899	1.00 29.62	В	C
45	ATOM	2294	CD1			-1.977	24.215	20.480	1.00 32.78 1.00 24.58	B B	c
	ATOM	2295	C		B 157 B 157	1.016	21.934 21.436	22.936 24.060	1.00 24.58	B	ŏ
	ATOM	2296 2297	O N	LEU		2.141	22.320	22.353	1.00 23.27	В	N
	ATOM	2298	CA		B 158	3.426	22.158	23.020	1.00 22.00	В	C
50	ATOM	2299	CB	LEU		3.933	20.721	22.832	1.00 22.79	В	С
	ATOM	2300	CG	LEU		3.978	20.154	21.407	1.00 26.19	B B	C
	ATOM	2301		LEU		5.220	20.663	20.676	1.00 25.77 1.00 24.53	В	c
	ATOM	2302	CD2	LEU		3.991 4.438	18.632 23.165	21.463	1.00 24.53	B	č
55	ATOM	2303 2304	0	LEU	B 158	4.118	24.000	21.648	1.00 19.23	В	ō
55	MOTA	2305	N	ALA	B 159	5.660	23.106	23.005	1.00 18.97	В	N
	ATOM	2306	CA	ALA	B 159	6.695	24.016	22.552	1.00 16.46	В	С
	ATOM	2307	CB	ALA	в 159	7.183	24.864	23.705	1.00 13.97	В	C
								01 067	1 00 16 E1	В	c
60	ATOM	2308 2309	C	ALA	B 159 B 159	7.826 8.214	23.189	21.967 22.536	1.00 16.51	B	Ö
	ATOM	2309	N	LEU		8.330	23.614	20.813	1.00 16.01	В	N
	ATOM	2310	CA	LEU		9.419	22.914	20.143	1.00 17.40	В	С
	ATOM	2312	CB	LEU		9.002	22.524	18.712	1.00 19.02	В	C
65	MOTA	2313	CG		B 160	10.016	21.678	17.928	1.00 20.39	В	C
	MOTA	2314	CD		B 160	10.062	20.269	18.520	1.00 21.64	B	C
	MOTA	2315	CD2		B 160 B 160	9.628 10.648	21.606	16.459 20.092	1.00 21.97	В	c
	ATOM ATOM	2316 2317	c		B 160	10.582	24.930	19.581	1.00 17.75	В	ő
70		2317	N		B 161	11.766	23.351	20.629	1.00 18.51	B	N
70	ATOM	2319	CA		B 161	13.002	24.136	20.624	1.00 19.34	В	C
	MOTA	2320	CB	LYS	в 161	13.612	24.188	22.039	1.00 19.45	В	С

-77-2321 14.832 25.113 22.166 1.00 20.17 A/T/OM CG LYS B 161 1.00 20.81 ATOM 2322 CD LYS B 161 15.129 25.442 23.625 В C 26.407 23.767 1.00 22.49 В ATOM 2323 CE LYS B 161 16.291 16.427 26.941 25.152 1.00 23.30 ATOM 2324 NZ LYS B 161 19.637 1.00 19.59 5 ATOM 2325 C LYS B 161 13.987 23.520 14.296 1.00 20.16 2326 LYS B 161 22.329 19.708 B MOTA 0 1.00 19.67 В ATTOM: N VAL B 162 14.471 24.336 18.709 17.688 1.00 21.10 2328 CA VAL B 162 15.402 23.867 В c MOTA 1.00 22.26 ATOM 2329 CB VAL B 162 14.945 24.292 16.276 1.0 ATOM VAL B 162 15.832 23.623 15.235 1.00 24.01 В 2330 CG1 13.465 23.934 16.058 1.00 22.27 В ATOM 2331 CG2 VAL B 162 1.00 21.17 ċ VAL B 162 16.800 24.430 17.908 в ATOM 2332 C 1.00 19.86 в ò ATOM 2333 0 VAL B 162 16.993 25.642 17.848 1.00 21.64 2334 N **LEU B 163** 17.768 23.544 18.133 в N ATOM 15 ATOM 2335 CA LEU B 163 19.157 23.950 18.369 1.00 20.49 B 23.326 19.670 1.00 20.44 в C CB LEU B 163 19.651 ATOM 2336 23.620 1.00 22.02 20.912 В С ATOM 2337 CG LEU B 163 18.813 19.087 22.573 21.978 1.00 22.74 в C **МОТ** 4 2338 CD1 LEU B 163 ATOM 2339 CD2 LEU B 163 19.121 25.026 21.417 1.00 22.92 C 20 ATOM 23.542 17.234 1.00 21.79 В c 2340 C LEU B 163 20.094 B ò ō LEU B 163 19.998 22.422 16.707 1.00 22.08 ATOM 2341 1.00 22.17 R N PHE B 164 21.008 24.441 16.861 A TOM 2342 N 15.795 1.00 22.32 В С ATOM 2343 CA PHE B 164 21.968 24.157 1.00 23.92 22.261 C ATOM 2344 CB PHE B 164 25.419 14.985 B 14.256 25 ATOM CG PHE B 164 21.063 25.946 1.00 30.95 C 2345 20.081 26.667 14.934 1.00 30.56 1.00 31.82 в č MOTA 2346 CD1 PHE B 164 ċ MOTA PHE B 164 20.880 25.668 12.903 R 2347 CD2 1.00 32.58 R c PHE B 164 18.935 27.099 14.281 MOTA 2348 CEL 12.238 1.00 34.84 C 2349 CE2 PHE B 164 19.733 26.096 ATOM 1.00 34.24 30 ATOM 2350 CZ PHE B 164 18.758 26.813 12.930 В PHE B 164 23.251 23.598 16.382 1.00 22.61 в C ATOM 2351 C 24.261 17.176 1.00 22.86 В 0 ATOM 2352 o PHE B 164 23.925 1.00 22.67 LYS B 165 23.582 22.371 15.994 В 747 ATOM 2353 N LYS B 165 24.777 21.711 16.511 1.00 22.73 С MOTA 2354 CA 1.00 21.42 15.827 24.982 20.360 35 ATOM 2355 CB LYS B 165 1.00 21.02 B c ATOM 2356 CG LYS B 165 24.153 19.240 16.419 2357 CD LVS B 165 24.153 18,010 15.506 1.00 22.54 В MOTA 16.926 16.062 1.00 22.64 в č ATOM 2358 CE LYS B 165 23.243 1.00 21.04 N ATOM 2359 NZ LYS B 165 23,231 15,701 15.230 В 16.388 40 ATOM LYS B 165 26.051 22.533 1.00 23.20 R 2360 C В Ó T.VS B 165 26.865 22.548 17.312 1.00 21.71 ATOM 2361 0 1.00 22.64 В N ATOM 2362 N ALA B 166 26.215 23.219 15,261 ATOM 2363 CA ALA B 166 27.416 24.013 15.026 1.00 24.25 В C ALA B 166 24.629 13.613 1.00 24.20 в C MOTA 2364 CB 27.384 1.00 24.80 č 45 ATOM 25.098 16.072 В 2365 C ALA B 166 27.636 ALA B 166 28.772 25.333 16.491 1.00 24.79 B 0 ATOM 2366 0 1.00 25.16 в N GLN B 167 26.563 25.758 16.495 ATOM 2367 N 1.00 26.89 17.503 B c MOTA 2368 CA GLN B 167 26.684 26.810 MOTA 2369 CB GLN B 167 25.411 27.660 17.545 1.00 29.97 R С 50 ATOM GLN B 167 25.203 28,462 18.834 1.00 37.08 В С 2370 CG 19.035 1.00 42.68 GLN B 167 29.587 MOTA 2371 CD 26.215 1.00 43.86 OE1 GLN B 167 27.425 29.351 19.185 R 0 алом 2372 1.00 43.02 R N NE2 GLN B 167 25.719 30.824 19.042 ATOM 2373 18.866 1.00 26.35 ATOM 2374 c GT.N B 167 26.950 26.193 55 ATOM 2375 ò **GLN B 167** 27.707 26.739 19.672 1.00 24.45 B a LEU B 168 25.041 24.339 1.00 25.56 B N 2376 N 26.334 19.111 ATOM 1.00 24.45 26.501 20 374 В ATOM 2377 CA LEU B 168 25.605 23.091 20.428 1.00 21.23 ъ ATOM 2378 CB LEU B 168 LEU B 168 24.076 23,257 20.548 1.00 24.32 В атом 2379 CG 1.00 19.55 60 ATOM 2380 CD1 LEU B 168 23.398 21.885 20.478 2381 cm2 LEU B 168 23.711 23.942 21.856 1.00 19.17 B c MOTA 1.00 25.52 В 2382 c LEU B 168 27.951 23.931 20.610 MOTA 28.501 21.674 1.00 23.62 B ATOM 2383 0 LEU B 168 24.192 1.00 27.52 В ATOM 2384 N **GLU B 169** 28.577 23.303 19.623 c 65 ATOM CA GLU B 169 29.948 22.844 19.809 1.00 32.03 R 2385 21.672 c ATOM 2386 CB GLII B 169 30.259 18.863 1.00 32.00 1.00 35.49 2387 CG GLU B 169 29.545 21.711 17.535 ATOM 16.954 1.00 35.75 2388 CD GLU B 169 29.317 20.317 MOVE 17.621 1.00 36.56 OR1 GLU B 169 28.662 19.485 MOTA 2389 1.00 34.75 15.829 ATOM 2390 OE2 GLU B 169 29.789 20.057 ċ 23.924 19.703 1.00 32.42 В АТОМ 2391 C GLII B 169 31.007 GLU B 169 32.114 23.762 20.202 1.00 34.46

ATOM 2392 0

							-78-				
	ATOM	2393	N	T.VQ	B 170	30.659	25.034	19.071	1.00 34.54	В	N
	ATOM	2394	CA	LYS	B 170	31.585	26.142	18.934	1.00 34.41	В	C
	ATOM	2395	CB	LYS	B 170	31.124	27.071	17.813	1.00 37.50	В	č
	ATOM	2396	CG	LYS	B 170	32.090	28.190	17.512	1.00 41.65	В	č
5	ATOM	2397	CD	LYS	B 170	31.700	28.922	16.240	1.00 45.85	В	C
	ATOM	2398	CE	LYS	B 170	31.944	28.064	15.005	1.00 48.44	В	C
	MOTA	2399	NZ	LYS	B 170	33.402	27.794	14.811	1.00 48.66	В	N
	ATOM	2400	С	LYS	B 170	31.639	26.899	20.253	1.00 34.06	В	C
10	ATOM MOTA	2401 2402	0	LYS	B 170	32.694	27.395	20.651	1.00 31.09	В	0
10	ATOM	2402	N CA	ALA	B 171 B 171	30.496 30.394	26.966 27.671	20.937	1.00 33.89	B	C
	ATOM	2404	CB	ALA	B 171	28.955	28.087	22.467	1.00 31.71	В	č
	ATOM	2405	c	ALA	B 171	30.914	26.869	23.398	1.00 36.33	В	č
	ATOM	2406	ō	ALA	B 171	30.973	27.374	24.517	1.00 37.82	В	ŏ
15	ATOM	2407	N	GLY	B 172	31.288	25.619	23.168	1.00 37.10	В	N
	ATOM	2408	CA	GLY	B 172	31.796	24.824	24.265	1.00 39.08	В	C
	ATOM	2409	C	GLY	B 172	31.293	23.408	24.199	1.00 41.69	В	C
	ATOM	2410	0	GLY	B 172	30.945	22.814	25.231	1.00 41.29	В	0
20	ATOM	2411	N CA	VAL	B 173 B 173	31.262	22.884	22.972	1.00 44.30	В	N
20	ATOM	2413	CB	VAL	B 173	30.807 31.989	21.528 20.572	22.670 22.425	1.00 44.96 1.00 46.41	B	C
	ATOM	2414	CG1	VAL	B 173	31.476	19.285	21.791	1.00 45.74	В	c
	ATOM	2415	CG2	VAL	B 173	33.048	21.246	21.539	1.00 44.74	В	č
	MOTA	2416	C	VAL	B 173	29.984	20.983	23.817	1.00 46.17	В	ċ
25	MOTA	2417	0	VAL	B 173	30.498	20.247	24.667	1.00 46.81	В	ō
	ATOM	2418	N	GLU	B 174	28.705	21.352	23.842	1.00 44.84	В	N
	MOTA	2419	CA	GLU	B 174	27.841	20.912	24.911	1.00 42.70	В	C
	ATOM	2420	CB	GLU	B 174	26.509	21.646	24.865	1.00 43.75	В	C
30	ATOM ATOM	2421	CG	GLU	B 174 B 174	26.485 27.483	22.871	25.754 25.329	1.00 44.96 1.00 45.73	B B	C
50	ATOM	2423	OE1	GLU	B 174	28.664	23.587	25.115	1.00 45.73	В	0
	ATOM	2424	OE2	GLU	B 174	27.087	25.108	25.219	1.00 45.36	В	ő
	ATOM	2425	C	GLU	B 174	27.611	19.420	24.997	1.00 42.19	В	č
	ATOM	2426	0	GLU	B 174	26.665	18.869	24.427	1.00 39.51	В	ō
35	ATOM	2427	N	HIS	B 175	28.522	18.781	25.719	1.00 41.13	В	N
	ATOM	2428	CA	HIS	B 175	28.458	17.365	26.001	1.00 40.20	В	C
	ATOM	2429	CB	HIS	B 175	29.845	16.864	26.435	1.00 44.57	В	C
	MOTA MOTA	2430 2431	CG	HIS	B 175	29.880	15.420	26.837	1.00 49.02	В	Ç
40	ATOM	2431		HIS	B 175 B 175	30.422 29.305	14.337 14.954	26.228 28.001	1.00 50.48 1.00 51.44	B	N
40	ATOM	2433		HIS	B 175	29.490	13.648	28.001	1.00 51.08	B	C
	MOTA	2434		HIS	B 175	30.165	13.249	27.027	1.00 51.29	В	N
	MOTA	2435	C	HIS	B 175	27.493	17.408	27.185	1.00 37.70	В	c
	MOTA	2436	0	HIS	B 175	26.942	16.394	27.604	1.00 37.04	В	0
45	MOTA	2437	N	GLN	B 176	27.282	18.621	27.692	1.00 35.01	В	N
	MOTA	2438	CA	GLN	B 176	26.399	18.841	28.827	1.00 36.23	В	C
	ATOM ATOM	2439 2440	CB	GLN	B 176 B 176	26.846	20.066	29.624	1.00 37.61	B	C
	ATOM	2441	CD	GLN	B 176	27.133 27.294	21.297 22.516	28.819 29.710	1.00 41.69 1.00 46.57	В	C
50	ATOM	2442	OE1	GLN	B 176	27.841	23.549	29.298	1.00 49.05	B	ŏ
	ATOM	2443	NE2	GLN	B 176	26.807	22.406	30.942	1.00 47.86	В	N
	MOTA	2444	C	GLN	B 176	24.921	18.970	28.473	1.00 34.56	В	C
	MOTA	2445	0	GLN	B 176	24.063	18.678	29.299	1.00 34.08	В	0
	MOTA	2446	N	LEU	B 177	24.624	19.419	27.259	1.00 33.44	В	N
55	MOTA	2447 2448	CA	LEU	B 177 B 177	23.240	19.533	26.824	1.00 32.62	В	C
	MOTA	2448	CG	PEA	B 177	23.163 21.829	20.178	25.433 24.665	1.00 33.83	B	c
	MOTA	2450		LEU	B 177	21.552	18.815	24.084	1.00 35.05	В	c
	MOTA	2451		LEU	B 177	20.698	20.638	25.581	1.00 33.78	В	č
60	ATOM	2452	C	LEU	B 177	22.728	18.102	26.776	1.00 31.62	В	č
	MOTA	2453	0	LEU	B 177	21.561	17.826	27.057	1.00 30.39	В	ō
	MOTA	2454	N	ARG	B 178	23.624	17.188	26.425	1.00 30.82	В	N
	MOTA	2455	CA	ARG	B 178	23.265	15.784	26.357	1.00 32.73	В	C
ce	MOTA	2456	CB	ARG	B 178	24.380	14.979	25.698	1.00 33.93	В	C
65	MOTA	2457 2458	CD	ARG	B 178 B 178	24.492 25.654	15.194 14.398	24.207	1.00 39.47	B B	C
	MOTA	2458	NE	ARG	B 178	25.654 25.537	14.398	23.658	1.00 44.54	B	C N
	MOTA	2460	CZ	ARG	B 178	26.501	12.989	23.838	1.00 47.63	В	C
	MOTA	2461		ARG	B 178	27.651	12.476	23.302	1.00 49.75	В	N
70	MOTA	2462	NH2		в 178	26.316	10.835	24.192	1.00 49.72	В	N
	MOTA	2463	С	ARG	B 178	22.998	15.241	27.753	1.00 32.47	В	C
	MOTA	2464	0	ARG	B 178	21.976	14.597	27.995	1.00 33.18	В	0

-79-15.506 23.912 28.676 1.00 30.61 мота 2465 N ARG B 179 1.00 31.15 MOTA 2466 CA ARG B 179 23.729 15.016 30.030 В 24.965 15.320 30.880 1.00 34.46 ATOM 2467 CB ARG B 179 ARG B 179 26.228 14.641 30.359 1.00 39.50 АТОМ 2468 CG 26,988 13.929 31.471 1.00 43.76 5 ATOM 2469 CD ARG B 179 ATOM 2470 ME ARC B 179 26.134 13.031 32.253 1.00 49.01 В N 1.00 49.97 MOTA 2471 CZ. ARG B 179 25.409 12.036 31.746 11.793 ATOM 2472 NH1 ARG B 179 25.421 30.441 1.00 51.21 в И ATOM 2473 NH2 ARG B 179 24.668 11.280 32.547 1.00 50.28 B N 10 ATOM ARG B 179 22,489 15.644 30.637 1.00 27.71 2474 C 15.006 31.394 1.00 26.64 21,776 В O ATOM 2475 0 ARG B 179 1.00 27.23 GLU B 180 22.228 16.896 30.279 В N ATOM 2476 N 1.00 26.36 c MOTA 2477 CA GLU B 180 21.070 17.620 30.782 ATOM 2478 CB GLU B 180 21.163 19.080 30.346 1.00 27.40 в ċ 1.00 30.43 C 15 ATOM 2479 CG GLU B 180 20.452 20.047 31.271 R GLU B 180 20.951 19.961 32,708 1.00 33.04 C ATTOM 2480 CD 1.00 32.92 В 0 MOTA 2481 OE1 GLU B 180 22.178 20.114 32.934 20.114 19.739 33.613 В 0 ATOM 2482 OE2 GLU B 180 MOTA 2483 C GLU B 180 19.746 16.997 30.296 1.00 25.78 20 Атом 18.796 16.863 31.063 1.00 24.13 1.00 25.67 0 2484 0 GLU B 180 В 2485 N VAL B 181 19.693 16.612 29.023 В N ATOM 18.494 1.00 27.08 c CA VAL B 181 16.002 28.453 Δ·TPOM 2486 1.00 27.03 26.936 B ATOM 2487 CB VAL B 181 18.693 15.717 1.00 27.81 ATOM 2488 CG1 VAL B 181 17.566 14.856 26.405 В 25 ATOM 2489 CG2 VAL B 181 18.745 17,029 26.171 1.00 22.54 18,155 14.703 29.188 1.00 28.77 1.00 30.48 B C ATOM 2490 C VAL B 181 VAL B 181 17.000 14.452 29.536 В 0 ATOM 2491 0 1.00 30.16 M 2492 N **GLU B 182** 19.175 13.887 29.433 ATOM 1.00 29.83 1.00 34.09 R C ATOM 2493 CA GLU B 182 19.024 12.615 30.139 c ATOM 2494 CB GLU B 182 20.394 11.937 30.231 B MOTA 2495 CG GLU B 182 20.452 10.614 30.983 1.00 40.35 В C 10.092 31.105 1.00 45.37 В c MOTA 2496 CD GLU B 182 21.884 1.00 47.27 OE1 GLU B 182 22.072 8.979 31.646 R O MOTA 2497 OE2 GLU B 182 22.826 10.798 30.657 1.00 47.17 АТОМ 2408 1.00 28.60 GLU B 182 18.445 12.843 31.534 35 ATOM 2499 C 1.00 28.99 R MOTA 2500 ō GLU B 182 17.457 12.223 31.920 0 MOTA 2501 N TLR R 183 19.060 13.741 32,290 1.00 27.98 B N ILE B 183 18.593 14.056 33.636 1.00 28.08 В c ATOM 2502 CA 1.00 28.69 C MOTA 2503 CB ILE B 183 19,493 15.130 34.293 В č 40 ATOM 2504 CG2 ILE B 183 18.894 15.567 35.618 1.00 27.35 B 1.00 28.95 В ċ 2505 CGI ILE B 183 20.910 14.586 34.484 ATOM 1.00 30.67 В c MOTA 2506 CD1 ILE B 183 21.880 15.609 35.030 MOTA 2507 C ILE B 183 17.153 14.588 33.627 1.00 28.81 В c 16.275 14.072 34.321 1.00 27.77 B 0 MOTA 2508 0 TLE B 183 1.00 27.78 45 15.632 32.837 В N ATOM 2509 N GLN B 184 16.934 2510 CA GLN B 184 15.635 16.283 32.721 1.00 29.40 в C MOTA 31.677 **GLN B 184** 15.728 17.393 1.00 29.48 в c ATOM 2511 CB 1.00 33.57 ć ATOM 2512 CG GLN B 184 15.084 18.695 32.085 ATOM 2513 CD GLN B 184 15.767 19.331 33.274 1.00 34.49 В ċ 50 ATOM 19.449 34.344 1.00 34.49 В Ó 2514 OE1 GLN B 184 15.177 19.740 1.00 36.47 33.095 В N ATOM 2515 NE2 **GLN B 184** 17.021 GLN B 184 14.474 15.349 32.360 1.00 29.74 В ATOM 2516 C 1.00 29.32 B 2517 GLN B 184 13.377 15.473 32.899 ATIOM 0 31.455 1.00 30.43 алом 2518 N SER B 185 14.714 14.411 в N 1.00 31.44 55 ATOM 2519 CA SER B 185 13.659 13.497 31.024 B c 12.710 29.801 1.00 29.48 в С алом 2520 CB SER B 185 14.123 30.147 SER B 185 15.188 1.00 33.05 в MOTA 2521 OG 11.853 SER B 185 13.151 12.524 32.093 1.00 32.12 В ATOM 2522 C SER B 185 12.156 11.842 31.884 1.00 31.84 В 0 **А/ГОМ** 2523 0 1.00 33.65 60 ATOM 2524 N HTS B 186 13.818 12.463 33.237 В N MONA 2525 CA HIS B 186 13.391 11.564 34.305 1.00 34.39 в 34.781 1.00 36.84 ATTOM 2526 CB HIS B 186 14.582 10.731 в HIS B 186 15 052 9.729 33.773 1.00 39.30 В алом 2527 CG 1.00 40.21 32.893 ATOM 2528 CD2 HIS B 186 14.363 8.961 В 65 ATOM ND1 HIS B 186 16.384 9.432 33.581 1.00 39.62 в N 2529 ATIOM 2530 CE1 HTS B 186 16.497 8.528 32.623 1.00 42.04 В 1.00 42.20 MOTA 2531 NE2 HIS B 186 15,286 8.225 32.189 B N HIS B 186 12.758 12.295 35.487 1.00 34.27 В MOTA 2532 C HIS B 186 12.296 11.667 36.442 1.00 34.94 MOTA 2533 1.00 32.72 LEU B 187 12.745 13.621 35.423 В 70 ATOM 2534 N LEU B 187 12.162 14.441 36.476 1.00 31.38 В MOTA 2535 CA CB LEU B 187 12.798 15.835 36.466 1.00 30.82

ATOM 2536

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	ATOM	2537	CG	LEU	в 187	14.074	16.108	37.274	1.00 31.43	В	C
	ATOM	2538			B 187	14.997	14.911	37.294	1.00 32.58	В	C
	ATOM	2539			В 187	14.764	17.317 14.569	36.686 36.248	1.00 31.34 1.00 31.86	B	c
5	ATOM	2540 2541	C		B 187 B 187	10.659 10.214	14.797	35.121	1.00 30.47	В	ŏ
,	ATOM	2542	N		B 188	9.881	14.413	37.316	1.00 31.25	В	N
	ATOM	2543	CA		в 188	8.429	14.530	37.230	1.00 30.44	В	C
	ATOM	2544	CB		B 188	7.789	13.148	37.091	1.00 29.88	В	C
10	ATOM	2545	C	ALA		7.912	15.237	38.481	1.00 29.21 1.00 28.34	В	C
10	MOTA	2546 2547	O N	ALA	B 188 B 189	7.862 7.538	14.651 16.504	39.559 38.319	1.00 28.72	B B	N
	ATOM	2548	CA		B 189	7.032	17.326	39.412	1.00 27.13	В	c
	ATOM	2549	CB		B 189	8.205	17.925	40.201	1.00 27.59	В	C
	MOTA	2550	CG		B 189	7.799	18.662	41.442	1.00 24.39	В	C
15	MOTA	2551			B 189	7.993	18.377	42.752	1.00 25.28	B B	C
	MOTA MOTA	2552 2553			B 189 B 189	7.122 6.919	19.859 20.283	41.410	1.00 26.03 1.00 24.93	В	C
	ATOM	2554			B 189	7.438	19.402	43.479	1.00 23.51	В	N
	ATOM	2555	C		B 189	6.193	18.431	38.787	1.00 26.49	В	C
20		2556	0		B 189	6.562	18.998	37.766	1.00 26.44	В	0
	MOTA	2557	N		B 190	5.049	18.760	39.402	1.00 26.98	B	N
	MOTA MOTA	2558 2559	CD		B 190 B 190	4.548	18.263 19.807	40.699 38.863	1.00 25.70 1.00 24.70	В	c
	ATOM	2560	CB		B 190	2.998	19.811	39.846	1.00 25.70	В	č
25	MOTA	2561	CG		в 190	3.633	19.382	41.139	1.00 26.97	В	C
	MOTA	2562	C		в 190	4.814	21.191	38.682	1.00 24.45	В	C
	ATOM	2563	0		B 190	4.378	21.966	37.832	1.00 24.60 1.00 22.38	B B	O
	MOTA MOTA	2564 2565	N CA	ASN	B 191 B 191	5.842 6.481	21.506	39.464 39.346	1.00 22.38	В	C
30	ATOM	2566	CB		B 191	6.713	23.408	40.730	1.00 21.05	В	č
	ATOM	2567	CG		B 191	5.436	23.575	41.495	1.00 19.72	В	C
	ATOM	2568			B 191	4.567	24.371	41.121	1.00 19.90	B	0
	ATOM	2569			B 191	5.299	22.815	42.571 38.564	1.00 20.48 1.00 21.58	B	N
35	ATOM	2570 2571	C		B 191 B 191	7.793 8.627	22.801	38.720	1.00 21.58	В	0
55	ATOM	2572	N		B 192	7.964	21.787	37.722	1.00 20.97	В	N
	ATOM	2573	CA	ILE	B 192	9.154	21.674	36.880	1.00 21.01	В	C
	ATOM	2574	CB		в 192	10.064	20.494	37.331	1.00 21.26	В	C
40	ATOM	2575	CG2		B 192 B 192	11.219 10.613	20.288	36.331 38.733	1.00 19.48 1.00 21.57	B B	C
40	ATOM	2576 2577	CD1		B 192	11.462	19.627	39.299	1.00 23.94	В	č
	ATOM	2578	c		в 192	8.667	21.432	35.453	1.00 19.86	В	C
	ATOM	2579	0		B 192	7.908	20.497	35.210	1.00 22.96	В	0
45	ATOM	2580	N		B 193	9.082	22,282	34.519 33.124	1.00 20.26 1.00 21.42	B	N C
43	ATOM	2581 2582	CA		B 193 B 193	8.669 9.307	22.142	32.268	1.00 21.42	В	č
	ATOM	2583	CG		B 193	8.681	23.436	30.883	1.00 23.28	В	C
	ATOM	2584			B 193	7.245	23.930	31.030	1.00 21.92	В	C
	ATOM	2585			B 193	9.495	24.445	30.101	1.00 19.52	В	C
50	ATOM	2586 2587	C		B 193 B 193	9.041 10.199	20.763	32.565 32.598	1.00 21.67 1.00 18.44	B	0
	ATOM	2588	N		B 194	8.041	20.069	32.036	1.00 21.75	В	N
	ATOM	2589	CA		B 194	8.215	18.732	31.482	1.00 23.01	В	C
	ATOM	2590	CB		B 194	6.841	18.096	31.268	1.00 25.81	В	C
55	MOTA	2591	CG		B 194	6.788	16.596	31.448	1.00 32.81	B	C
	MOTA	2592 2593	CD		B 194 B 194	6.817 6.281	16.240 14.904	33.176	1.00 44.90	В	N
	ATOM	2594	CZ		B 194	5.012	14.542	32.974	1.00 47.96	В	Ĉ
	ATOM	2595			B 194	4.125	15.418	32.508	1.00 48.71	В	N
60	MOTA	2596			в 194	4.626	13.299	33.247	1.00 48.22	B	N
	MOTA	2597	C		B 194	8.981	18.673	30.159	1.00 21.93	B	C
	MOTA	2598 2599	O.		B 194 B 195	8.821 9.819	19.538 17.647	29.292 30.021	1.00 19.59 1.00 21.33	В	N
	ATOM	2600	CA		B 195	10.567	17.403	28.788	1.00 22.76	В	C
65	MOTA	2601	CB	LEU	B 195	12.053	17.148	29.069	1.00 22.81	В	C
	ATOM	2602	CG		B 195	13.078	17.437	27.959	1.00 24.02	В	C
	MOTA	2603			B 195	14.267	16.498	28.140 26.563	1.00 21.85 1.00 23.51	B B	C
	ATOM	2604 2605	CD2		B 195 B 195	12.483 9.921	17.251 16.119	28.274	1.00 23.31	В	c
70	ATOM	2606	ö		B 195	10.110	15.056	28.861	1.00 22.57	В	0
	ATOM	2607	N	TYR	в 196	9.145	16.215	27.201	1.00 22.31	В	N
	ATOM	2608	CA	TYR	В 196	8.453	15.050	26.651	1.00 22.19	В	C

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	ATOM	2609	СВ	TYR	в	196	7.281	15.490	25.768	1.00 2	33.58	3	3	c
	ATOM	2610	CG	TYR		196	6.155	16.146	26.519	1.00 2		1		C
	ATOM	2611	CD1	TYR		196	5.772	17.460	26.238	1.00 2		3		C
_	ATOM	2612	CE1	TYR		196	4.728	18.071	26.937		24.87	1		c
5	ATOM	2613		TYR		196	5.467 4.426	15.457 16.056	27.515 28.217	1.00 2				c
	ATOM	2614 2615	CE2	TYR		196 196	4.062	17.361	27.923	1.00 2	25.01			c
	ATOM	2616	OH	TYR		196	3.023	17.944	28.612	1.00 2	29.27	i		ō
	ATOM	2617	c	TYR		196	9.333	14,108	25.851	1.00 2	22.57	1	3	С
10	ATOM	2618	0	TYR		196	9.132	12.898	25.873	1.00 2		1		0
	ATOM	2619	N	GPA		197	10.294	14.663	25.124	1.00 2		1		N
	ATOM	2620	CA	GLY		197	11.180	13.841	24.332	1.00		1		C
	ATOM	2621 2622	C	GLY		197 197	12.161 12.220	14.702 15.919	23.572 23.772	1.00		i		Ö
15	ATOM	2623	N	TYR		198	12.935	14.078	22.695	1.00		i		N
15	ATOM	2624	CA	TYR		198	13.903	14.810	21.900	1.00		1		C
	ATOM	2625	CB	TYR		198	15.140	15.125	22.735	1.00	31.42	1		C
	ATOM	2626	CG	TYR		198	15.966	13.915	23.087	1.00			3	C
	ATOM	2627		TYR		198	17.100	13.584	22.349	1.00		1		C
20	MOTA	2628	CE1			198	17.863	12.466 13.096	22.667 24.158	1.00			B B	C
	ATOM ATOM	2629 2630	CD2 CE2	TYR		198 198	15.611 16.364	11.977	24.136	1.00			3	č
	ATOM	2631	CZ	TYR		198	17.489	11.667	23.734	1.00			В	č
	ATOM	2632	OH	TYR		198	18.232	10.550	24.049	1.00		:	В	0
25	ATOM	2633	С	TYR		198	14.293	13.982	20.699	1.00			В	C
	ATOM	2634	0		в	198	13.951	12.812	20.611	1.00			В	0
	MOTA	2635	N		В	199	15.000	14.599	19.767	1.00			B B	N C
	ATOM	2636 2637	CA		В	199 199	15.443 14.233	13.904 13.426	18.572 17.749	1.00			В	č
30	ATOM	2638	CG	PHE			13.388	14.540	17.161	1.00			В	č
-	ATOM	2639		PHE			13.637	15.019	15.876	1.00			В	C
	ATOM	2640	CD2	PHE			12.310	15.064	17.868	1.00			В	C
	ATOM	2641		PHE			12.824	15.996	15.301	1.00			В	С
25	ATOM	2642		PHE			11.492	16.040	17.303 16.015	1.00			B B	C
35	ATOM ATOM	2643 2644	CZ	PHE			11.750 16.297	16.505 14.860	17.767	1.00			В	č
	ATOM	2645	o	PHE			16.345	16.049	18.073	1.00			В	ŏ
	ATOM	2646	N	HIS	В	200	16.993	14.353	16.758	1.00			В	N
	MOTA	2647	CA	HIS			17.806	15.238	15.938	1.00			В	C
40	ATOM	2648	CB	HIS			19.100	15.594	16.681	1.00	33.26		B B	C
	ATOM	2649 2650	CG	HIS			19.948 21.287	14.418 14.230	17.048 16.965	1.00			В	c
	ATOM ATOM	2651		HIS			19.439	13.288	17.648	1.00			В	N
	ATOM	2652		HIS			20.427	12.454	17.921	1.00	37.18		В	C
45	ATOM	2653	NE2	HIS	в	200	21.559	13.003	17.517	1.00	36.60		В	N
	ATOM	2654	С	HIS			18.116	14.715	14.538	1.00			В	C
	ATOM	2655	0	HIS			17.752	13.591	14.187	1.00			В	O N
	ATOM	2656 2657	N CA	ASP			18.725 19.138	15.571 15.186	13.721 12.377	1.00			В	C
50	ATOM	2658	CB			201	18.335	15.916	11.282	1.00			В	č
	ATOM	2659	CG			201	18.264	17.424	11.483	1.00	25.88		В	C
	ATOM	2660				201	19.294	18.047	11.802	1.00			В	0
	MOTA	2661	OD2			201	17.166	17.998	11.290	1.00			В	C
55	MOTA	2662	C	ASP			20.627 21.263	15.505 15.653	12.299	1.00			B B	0
33	ATOM ATOM	2663 2664	N	ALA			21.184	15.617	11.096	1.00			В	N
	ATOM	2665	CA	ALA			22.615	15.887	10.946	1.00			В	C
	ATOM	2666	CB	ALA	В	202	23.038	15.661	9.485	1.00			В	C
	ATOM	2667	С	ALA			23.106	17.263	11.420	1.00			В	С
60	MOTA	2668	0	ALA			24.289	17.437	11.710	1.00			В	O
	ATOM	2669	N	ALA ALA			22.212 22.654	18.237 19.564	11.520 11.935	1.00			B B	C
	ATOM	2670 2671	CB	ALA			22.654	20.502	10.718	1.00	18.98		В	č
	ATOM	2672	CB	ALA			21.902	20.213	13.095	1.00			В	č
65	ATOM	2673	ŏ	ALA		203	22.321	21.262	13.583	1.00	19.24		В	0
	ATOM	2674	N	ARG	В	204	20.825	19.595	13.568	1.00	17.86		В	N
	ATOM	2675	CA	ARG			20.060	20.197	14.660	1.00			В	C
	MOTA	2676	CB	ARG			18.849 19.083	20.964	14.111	1.00			B B	C
70	ATOM	2677 2678	CD.	ARG			17.793	22.345	12.813	1.00			В	č
, 0	ATOM	2679	NE.	ARG			17.847	22.663	10.890	1.00			В	N
	ATOM	2680	CZ	ARG			17.679	21.773	9.911	1.00			В	C

							-82-				
	ATOM	2681		ARG I		17.752	22.161	8.644	1.00 41.01	В	N
	ATOM	2682		ARG 1		17.419	20.500	10.191	1.00 38.76	B B	N
	ATOM	2683 2684	C		3 204 3 204	19.547 19.463	19.228 18.030	15.711 15.492	1.00 18.39 1.00 18.56	B	0
5	ATOM	2685	N		3 204	19.199	19.767	16.870	1.00 18.68	В	N
,	ATOM	2686	CA		3 205	18.649	18.958	17.949	1.00 18.67	В	C
	ATOM	2687	CB		B 205	19.551	18.984	19.201	1.00 18.98	В	C
	ATOM	2688		VAL 1		18.933	18.135	20.301	1.00 19.79	В	C
10	MOTA	2689		VAL		20.947 17.290	18.472 19.572	18.852 18.282	1.00 15.84 1.00 19.14	B B	c
10	MOTA	2690 2691	C		3 205 B 205	17.182	20.796	18.405	1.00 21.54	В	0
	71011	2051	Ü	7,20	200	271202				_	
	ATOM	2692	N		B 206	16.263	18.731	18.396	1.00 17.89	B	N
	ATOM	2693	CA	TYR I		14.910	19.193	18.709	1.00 19.04	B B	C
15	ATOM	2694 2695	CB	TYR I		13.891 14.228	18.696 19.017	17.674 16.240	1.00 18.60 1.00 18.39	В	C
	ATOM	2696		TYR I		15.207	18.293	15.565	1.00 21.42	В	č
	ATOM	2697	CE1	TYR		15.542	18.578	14.244	1.00 21.55	В	C
	ATOM	2698	CD2	TYR :		13.576	20.052	15.555	1.00 19.46	В	C
20	ATOM	2699	CE2		B 206	13.907	20.352	14.216	1.00 21.97	В	C
	ATOM	2700 2701	OH		B 206 B 206	14.898 15.267	19.602 19.858	13.573 12.269	1.00 23.91 1.00 26.45	B B	o
	MOTA MOTA	2701	C		B 206	14.459	18.705	20.073	1.00 19.50	В	č
	MOTA	2703	ŏ		B 206	14.538	17.508	20.373	1.00 21.94	В	ō
25	MOTA	2704	N	LEU :	B 207	13.985	19.633	20.897	1.00 16.85	В	N
	ATOM	2705	CA		B 207	13.491	19.291	22.224	1.00 17.98	В	C
	ATOM	2706	CB		B 207	14.181	20.161	23.286	1.00 16.72	B	C
	ATOM ATOM	2707 2708	CG	LEU :	B 207	15.722 16.216	20.138	23.321 24.461	1.00 19.44 1.00 19.09	В	c
30	ATOM	2709		LEU		16.226	18.707	23.519	1.00 19.58	В	č
50	ATOM	2710	c	LEU		11.973	19.535	22.225	1.00 17.04	В	C
	ATOM	2711	Ö	LEU :	B 207	11.513	20.588	21.803	1.00 18.06	В	0
	MOTA	2712	N	ILE :		11.205	18.547	22.674	1.00 18.23	В	N
35	ATOM	2713 2714	CA	ILE :		9.747 9.093	18.653 17.336	22.727 22.272	1.00 16.54 1.00 16.55	B	C
55	ATOM	2714	CG2	ILE :		7.568	17.474	22.238	1.00 14.96	В	č
	ATOM	2716		ILE		9.614	16.978	20.872	1.00 20.37	В	C
	ATOM	2717	CD1			9.149	15.613	20.347	1.00 21.43	В	C
	MOTA	2718	C	ILE :		9.412	18.969	24.179	1.00 17.23	В	C
40		2719	N	LEU		9.636 8.871	18.144 20.166	25.081 24.401	1.00 16.63 1.00 16.12	B	N
	ATOM ATOM	2720 2721	CA	LEU		8.577	20.630	25.752	1.00 17.56	В	C
	ATOM	2722	CB	LEU		9.472	21.830	26.063	1.00 17.90	В	C
	ATOM	2723	CG	LEU	в 209	10.978	21.577	25.959	1.00 19.46	B	C
45	MOTA	2724	CD1	LEU		11.664	22.798	25.379	1.00 19.75	B B	c
	MOTA	2725	CD2		B 209 B 209	11.525 7.144	21.215 21.018	27.336 26.084	1.00 19.17 1.00 18.62	В	c
	MOTA	2726 2727	0		B 209	6.348	21.346	25.202	1.00 18.84	В	ŏ
	ATOM	2728	N		B 210	6.844	20.984	27.381	1.00 16.02	В	N
50		2729	CA	GLÜ	B 210	5.549	21.382	27.898	1.00 17.17	В	C
	ATOM	2730	CB		B 210	5.496	21.128	29.409	1.00 16.24	В	C
	ATOM	2731 2732	CC		B 210 B 210	4.275	21.705 21.542	30.100 31.615	1.00 17.66 1.00 19.26	B	c
	ATOM	2732	OE1		B 210	3.396	22.037	32.298	1.00 19.17	В	Ö
55	ATOM	2734	OE2		B 210	5.273	20.919	32.126	1.00 18.51	В	ō
	ATOM	2735	C		В 210	5.419	22.881	27.619	1.00 17.58	В	C
	ATOM	2736	0		в 210	6.386	23.640	27.787	1.00 17.15	В	0
	ATOM	2737	N		B 211	4.239	23.301	27.177 26.875	1.00 17.46 1.00 17.27	B B	N
60	MOTA	2738 2739	CA		B 211 B 211	3.975 2.915	24.707 24.830	25.771	1.00 17.32	В	č
00	ATOM	2740	CG		B 211	2.598	26.265	25.406	1.00 18.99	В	č
	ATOM	2741	CD1	TYR	B 211	3.601	27.115	24.953	1.00 18.89	В	C
	ATOM	2742	CE1		B 211	3.337	28.443	24.637	1.00 18.07	В	C
	ATOM	2743	CD2		B 211	1.300	26.783	25.536	1.00 19.53	B	C
65	ATOM	2744 2745	CE2		B 211 B 211	1.025 2.058	28.124 28.943	25.215 24.766	1.00 17.93 1.00 19.57	В	c
	ATOM	2745	OH		B 211	1.837	30.268	24.700	1.00 21.28	В	0
	MOTA	2747	c		B 211	3.488	25.437	28.119	1.00 17.08	В	С
	ATOM	2748	o		в 211	2.676	24.905	28.880	1.00 20.12	В	0
70		2749	N		в 212	3.977	26.657	28.315	1.00 16.19	В	N
	MOTA	2750	CA		B 212	3.619 4.882	27.487	29.470 30.202	1.00 16.51 1.00 15.30	B	C
	ATOM	2751	CB	min	B 212	4.082	27.927	30.202	1.00 15.50	ь	_

							-83-				
	ATOM	2752	C		B 212	2.856	28.705	28.952	1.00 17.50	В	C
	ATOM	2753	0		B 212	3.450	29.726	28.596	1.00 18.16	В	0
	MOTA MOTA	2754 2755	CD		B 213 B 213	1.520 0.728	28.618 27.494	28.925 29.458	1.00 17.93 1.00 16.26	B	N C
5	ATOM	2756	CA		B 213	0.651	29.693	28.437	1.00 18.73	В	č
-	ATOM	2757	CB		B 213	-0.758	29.108	28.604	1.00 17.80	В	c
	ATOM	2758	CG		B 213	-0.609	28.146	29.724	1.00 19.64	В	C
	MOTA	2759	C		B 213	0.761	31.115	28.984	1.00 19.83	В	C
	MOTA	2760	0		B 213	0.513	32.063	28.245	1.00 20.80	В	0
10	ATOM	2761	N		B 214	1.128	31.288	30.250	1.00 20.66	B	N
	ATOM	2762 2763	CA		B 214 B 214	1.211	32.640 32.647	30.798 32.255	1.00 20.06 1.00 19.58	В	C
	ATOM	2764	œ		B 214	-0.812	32.790	32.467	1.00 22.04	В	c
	ATOM	2765			B 214	-1.576	31.829	31.576	1.00 23.11	В	ċ
15	ATOM	2766	CD2	LEU	B 214	-1.161	32.538	33.926	1.00 22.72	В	C
	MOTA	2767	C		B 214	2.572	33.346	30.686	1.00 21.48	В	C
	ATOM	2768	0		B 214	2.749	34.451	31.200	1.00 23.25 1.00 21.00	B	0
	ATOM	2769 2770	N CA		B 215 B 215	3.533 4.825	32.724 33.368	30.013 29.847	1.00 21.00	В	N
20	ATOM	2771	CA		B 215	5.790	33.300	31.023	1.00 23.13	В	č
	ATOM	2772	ŏ		B 215	5.657	32.448	31.904	1.00 23.73	В	ō
	MOTA	2773	N		B 216	6.758	34.214	31.042	1.00 22.29	В	N
	ATOM	2774	CA		B 216	7.779	34.238	32.088	1.00 23.81	В	C
25	MOTA	2775	CB		B 216	9.127 9.090	34.692	31.517	1.00 23.63 1.00 25.10	B B	C
23	ATOM ATOM	2776 2777			B 216 B 216	9.409	36.102 33.987	31.277 30.199	1.00 23.10	В	č
	ATOM	2778	C		B 216	7.461	35.125	33.291	1.00 23.33	В	č
	ATOM	2779	ŏ		B 216	6.712	36.100	33.191	1.00 20.98	В	ō
	ATOM	2780	N		B 217	8.036	34.774	34.435	1.00 22.90	В	N
30	MOTA	2781	CA		B 217	7.827	35.554	35.651	1.00 24.21	В	С
	MOTA	2782	CB		B 217 B 217	8.470 8.387	34.857 35.740	36.867 38.109	1.00 23.26	B	C
	ATOM ATOM	2783 2784			B 217	7.763	33.552	37.110	1.00 22.25	В	c
	ATOM	2785	C		B 217	8.439	36.935	35.449	1.00 23.65	В	č
35	ATOM	2786	ō		в 217	7.922	37.933	35.932	1.00 23.81	В	0
	ATOM	2787	N		B 218	9.536	36.967	34.708	1.00 25.98	В	N
	ATOM	2788	CA		B 218	10.247	38.193	34.395	1.00 29.23	В	C
	ATOM	2789 2790	CB		B 218 B 218	11.395 12.225	37.865 39.040	33.437 32.974	1.00 33.60 1.00 37.23	B B	C
40	ATOM	2791			B 218	11.965	39.661	31.753	1.00 37.23	В	č
	ATOM	2792			B 218	12.756	40.710	31.296	1.00 40.90	В	Ċ
	ATOM	2793			B 218	13.296	39.503	33.733	1.00 39.21	В	C
	ATOM	2794			B 218	14.096	40.551	33.285	1.00 41.41	В	C
45	ATOM	2795	CZ		B 218	13.819	41.149	32.065 31.607	1.00 42.06 1.00 43.77	B B	C
45	ATOM ATOM	2796 2797	OH		B 218 B 218	14.609 9.302	42.175 39.228	33.788	1.00 30.16	В	c
	ATOM	2798	ŏ		B 218	9.259	40.368	34.242	1.00 31.95	В	ŏ
	ATOM	2799	N		B 219	8.540	38.831	32.770	1.00 30.65	В	N
	ATOM	2800	CA		B 219	7.589	39.736	32.123	1.00 29.66	В	C
50	ATOM	2801	CB		B 219	6.906	39.026	30.967	1.00 28.94	В	C
	ATOM ATOM	2802 2803	C		B 219 B 219	6.542 6.199	40.257	33.118 33.110	1.00 29.78 1.00 28.08	B B	C
	ATOM	2804	N		B 220	6.027	39.371	33.964	1.00 30.79	В	N
	ATOM	2805	CA		B 220	5.037	39.753	34.968	1.00 34.09	В	C
55	ATOM	2806	CB		B 220	4.587	38.529	35.766	1.00 36.73	В	C
	ATOM	2807	CG		в 220	3.344	37.838	35.251	1.00 43.32	В	C
	ATOM	2808	CD		B 220 B 220	2.073 1.801	38.618	35.542	1.00 46.85 1.00 48.71	B B	c
	ATOM ATOM	2809 2810			B 220	1.350	39.613 38.237	36.489	1.00 48.33	В	ő
60	ATOM	2811	C		B 220	5.618	40.785	35.934	1.00 34.92	В	č
	ATOM	2812	o	GLU	B 220	4.956	41.755	36.296	1.00 36.60	В	0
	ATOM	2813	N		B 221	6.858	40.569	36.356	1.00 34.26	В	N
	MOTA	2814	CA		B 221	7.505	41.482	37.286	1.00 34.78	В	C
65	ATOM	2815	CB		B 221	8.920	40.995	37.621	1.00 33.24	B B	c
03	MOTA	2816 2817	CD1		B 221 B 221	9.646 8.807	41.761	38.735 40.010	1.00 32.72 1.00 30.46	В	C
	ATOM	2818			B 221	10.996	41.112	38.988	1.00 32.35	В	C
	MOTA	2819	c		B 221	7.565	42.880	36.693	1.00 34.90	В	С
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70	ATOM	2820	O N		B 221	7.275	43.864	37.374	1.00 32.14	B	N
	MOTA	2821 2822	CA		B 222 B 222	7.941 8.026	42.961 44.241	35.419 34.735	1.00 35.21 1.00 37.12	В	C
	WIOH	2002	CA	السدى	- 006	0.020	44.441	34.133	2.00 37.12		_

							-84-				
	MOTA	2823 2824	CB		B 222 B 222	8.563 9.945	44.044	33.319	1.00 39.87	В	C
	ATOM	2825	CD		B 222	10.690	43.424	33.287 32.004	1.00 44.00 1.00 47.25	B B	c
-	MOTA	2826	OE1		B 222	10.220	43.410	30.907	1.00 49.30	В	ō
5	ATOM	2827 2828	NE2 C	GLN		11.864 6.684	44.333	32.135 34.687	1.00 48.03	В	N
	ATOM	2829	ö	GLN		6.634	46.184	34.865	1.00 36.68 1.00 37.49	B B	C
	ATOM	2830	N	LYS	B 223	5.597	44.241	34.461	1.00 35.79	В	N
10	ATOM	2831 2832	CB		B 223 B 223	4.277 3.237	44.859 43.868	34.406	1.00 36.52 1.00 37.92	B B	C
10	ATOM	2833	CG		B 223	3.354	43.561	32.389	1.00 37.92	В	C
	MOTA	2834	CD	LYS	B 223	2.292	42.560	31.944	1.00 42.68	В	C
	ATOM ATOM	2835 2836	CE		B 223 B 223	0.886	43.140	32.033	1.00 43.66	В	C
15	ATOM	2837	C		B 223	0.693 3.792	44.275 45.402	31.079 35.749	1.00 46.03 1.00 36.84	B	N
	MOTA	2838	0	LYS	B 223	3.357	46.550	35.833	1.00 38.21	В	Ö
	MOTA	2839	N		B 224	3.860	44.580	36.795	1.00 35.10	В	N
	ATOM	2840 2841	CA		B 224 B 224	3.398 2.929	44.988	38.122 38.913	1.00 33.56 1.00 33.55	B	C
20	ATOM	2842	CG		B 224	1.871	42.852	38.282	1.00 34.89	В	c
	ATOM	2843	CD1		B 224	1.619	41.658	39.189	1.00 33.24	В	C
	ATOM	2844 2845	CD2		B 224 B 224	0.589 4.452	43.630 45.735	38.059 38.939	1.00 34.60	В	C
	ATOM	2846	ŏ		B 224	4.141	46.297	39.989	1.00 32.05 1.00 32.92	B	C
25	ATOM	2847	N	SER	B 225	5.691	45.723	38.455	1.00 30.59	В	N
	ATOM	2848	CA		B 225	6.826	46.380	39.112	1.00 31.41	В	C
	ATOM	2849 2850	CB OG		B 225 B 225	6.449 7.615	47.792 48.537	39.549 39.843	1.00 32.21 1.00 34.55	B	0
	ATOM	2851	C	SER	B 225	7.361	45.585	40.318	1.00 31.23	B	č
30	ATOM	2852	0		B 225	8.556	45.589	40.599	1.00 30.58	В	0
	ATOM	2853 2854	N CA		B 226 B 226	6.466 6.851	44.921 44.096	41.035	1.00 30.59 1.00 31.60	B	N
	ATOM	2855	CB		B 226	7.535	44.924	43.273	1.00 31.60	В	C
25	MOTA	2856	CG	LYS	B 226	6.733	46.065	43.866	1.00 33.34	В	C
35	MOTA	2857 2858	CD	LYS	B 226 B 226	7.482 6.839	46.606 47.858	45.085 45.658	1.00 37.58 1.00 39.62	В	C
	MOTA	2859	NZ	LYS	B 226	7.074	49.049	44.786	1.00 39.62	B	C
	MOTA	2860	C	LYS	B 226	5.620	43.400	42.707	1.00 29.47	В	č
40	MOTA MOTA	2861 2862	O N	LYS	B 226 B 227	4.501 5.821	43.795	42.391	1.00 29.83	В	0
70	ATOM	2863	CA	PHE		4.702	42.355 41.597	43.500	1.00 28.21 1.00 26.85	B	N
	ATOM	2864	CB	PHE	B 227	4.928	40.091	43.833	1.00 28.42	В	č
	ATOM ATOM	2865	CG		B 227	5.401	39.718	42.453	1.00 27.26	В	c
45	ATOM	2866 2867		PHE		4.884 6.352	40.346 38.712	41.321	1.00 27.70	B B	c
	ATOM	2868	CE1	PHE	B 227	5.308	39.976	40.041	1.00 27.47	В	č
	ATOM	2869		PHE		6.786	38.334	41.011	1.00 27.41	В	C
	ATOM	2870 2871	CZ	PHE		6.261 4.453	38.969 41.850	39.887 45.525	1.00 27.84	B B	c
50	ATOM	2872	ŏ	PHE		5.307	42.385	46.229	1.00 25.45	В	0
	ATOM	2873	N	ASP		3.273	41.442	45.983	1.00 24.91	В	N
	ATOM	2874 2875	CB	ASP		2.870 1.346	41.576	47.375 47.484	1.00 25.21 1.00 25.97	B	C
	ATOM	2876	CG	ASP		0.675	40.479	46.742	1.00 26.97	В	č
55	ATOM	2877		ASP		0.468	40.611	45.525	1.00 33.21	В	0
	ATOM ATOM	2878 2879	OD2	ASP	B 228 B 228	0.373 3.394	39.440	47.359	1.00 27.04	В	0
	ATOM	2880	ö		B 228	3.979	40.357	48.129 47.528	1.00 26.47 1.00 26.50	B	C
	MOTA	2881	N	GLU	B 229	3.158	40.327	49.436	1.00 25.93	В	N
60	MOTA	2882 2883	CB		B 229 B 229	3.627 3.425	39.234	50.275	1.00 25.05	В	C
	ATOM	2884	CG	GLU		4.230	39.579 40.789	51.757 52.233	1.00 26.99 1.00 30.82	B	C
	ATOM	2885	CD		B 229	4.296	40.905	53.753	1.00 31.53	В	C
65	MOTA	2886	OE1	GLU		3.239	41.053	54.403	1.00 32.47	В	0
0.5	MOTA	2887 2888	OE2		B 229 B 229	5.415 2.961	40.847 37.900	54.299 49.973	1.00 33.80 1.00 25.00	B	0
	MOTA	2889	0	GLU	B 229	3.624	36.855	49.985	1.00 22.64	В	ö
	ATOM	2890	N		B 230	1.657	37.930	49.702	1.00 23.27	В	N
70	ATOM	2891 2892	CA		B 230 B 230	0.925 -0.577	36.698 36.990	49.420 49.254	1.00 25.73 1.00 30.97	B B	c
	ATOM	2893	CG	GLN		-1.443	35.736	49.254	1.00 30.97	В	C
	MOTA	2894	CD	GLN	B 230	-2.902	36.043	48.773	1.00 41.26	В	c

							-85-				
	ATOM	2895			B 230	-3.214	36.601	47.720	1.00 43.42	В	0
	MOTA	2896	NE2		B 230	-3.800	35.673	49.679	1.00 43.12	B B	N
	ATOM	2897 2898	C		B 230 B 230	1.477	36.003 34.811	48.173 48.203	1.00 22.96 1.00 22.41	В	0
5	ATOM	2899	N		B 231	1.618	36.750	47.081	1.00 21.69	В	N
-	ATOM	2900	CA		B 231	2.151	36.196	45.841	1.00 20.70	В	C
	ATOM	2901	CB		B 231	2.067	37.237	44.720	1.00 24.11	В	C
	ATOM	2902	CG		B 231	2.972	36.943	43.534	1.00 29.60	В	C
10	ATOM	2903	CD		B 231	2.207 1.381	36.654 37.776	42.261 41.827	1.00 32.47 1.00 35.86	B B	C
10	ATOM	2904 2905	NE CZ		B 231 B 231	1.031	37.776	40.562	1.00 38.81	В	C
	ATOM	2906	NH1		B 231	0.269	39.031	40.249	1.00 39.91	В	N
	ATOM	2907	NH2	ARG :	B 231	1.466	37.183	39.602	1.00 38.33	В	N
	ATOM	2908	C		B 231	3.606	35.719	46.001	1.00 19.50	В	С
15	ATOM	2909	0		B 231	3.957	34.622	45.557 46.635	1.00 17.71 1.00 17.49	B B	O N
	MOTA	2910 2911	N CA		B 232 B 232	4.441 5.838	36.538 36.184	46.847	1.00 17.49	В	C
	ATOM	2912	CB		B 232	6.612	37.312	47.576	1.00 19.54	В	č
	ATOM	2913	OG1		B 232	6.597	38.504	46.782	1.00 13.78	В	0
20	ATOM	2914	CG2		B 232	8.082	36.879	47.834	1.00 14.78	В	C
	ATOM	2915	С		B 232	5.956	34.904	47.682	1.00 17.18	В	C
	ATOM ATOM	2916 2917	O		B 232 B 233	6.672 5.243	33.984 34.852	47.307 48.807	1.00 15.09 1.00 19.12	B	N
	ATOM	2917	CA		B 233	5.243	33.684	49.695	1.00 18.94	В	C
25	ATOM	2919	CB		B 233	4.352	33.925	50.906	1.00 17.71	В	С
	ATOM	2920	C	ALA	B 233	4.828	32.407	48.966	1.00 19.02	В	С
	ATOM	2921	0		B 233	5.417	31.334	49.157	1.00 18.32	В	0
	ATOM	2922	N		В 234	3.785 3.275	32.527 31.399	48.148	1.00 19.42 1.00 18.40	B	И
30	MOTA	2923 2924	CA		B 234 B 234	1.975	31.784	46.620	1.00 17.88	В	č
50	ATOM	2925	OG1		B 234	0.965	32.134	47.575	1.00 15.16	В	0
	MOTA	2926	CG2		B 234	1.480	30.618	45.762	1.00 16.22	В	C
	MOTA	2927	C		B 234	4.329	30.932	46.364	1.00 18.28	В	С
20	ATOM	2928	0		B 234 B 235	4.550 4.981	29.735 31.876	46.196 45.694	1.00 20.75 1.00 19.08	B	O N
35	ATOM	2929 2930	N CA		B 235	6.034	31.540	44.736	1.00 19.08	В	C
	ATOM	2931	CB	TYR	B 235	6.514	32.803	44.014	1.00 19.29	В	č
	ATOM	2932	CG	TYR	B 235	5.661	33.258	42.851	1.00 21.57	В	С
	ATOM	2933	CD1		B 235	4.389	32.729	42.634	1.00 23.85	В	C
40		2934	CE1		B 235	3.589	33.176 34.247	41.579 41.984	1.00 24.93 1.00 21.08	B B	C
	ATOM ATOM	2935 2936	CD2 CE2		B 235 B 235	6.116 5.325	34.705	40.926	1.00 24.94	. в	č
	ATOM	2937	CZ		B 235	4.063	34.168	40.728	1.00 26.16	В	C
	ATOM	2938	OH		В 235	3.267	34.628	39.695	1.00 22.88	В	0
45	ATOM	2939	C		B 235	7.242	30.871	45.423	1.00 18.91	B B	C
	MOTA	2940 2941	O N		B 235 B 236	7.855 7.603	29.956 31.336	44.869 46.619	1.00 18.47 1.00 18.40	В	N
	ATOM ATOM	2941	CA		B 236	8.745	30.741	47.321	1.00 17.73	В	č
	ATOM	2943	CB		B 236	9.188	31.601	48.541	1.00 18.76	В	C
50	MOTA	2944	CG2		B 236	10.387	30.945	49.254	1.00 18.52	В	С
	MOTA	2945			B 236	9.612	32.999	48.065	1.00 19.28	В	C
	ATOM ATOM	2946 2947	CD1		B 236 B 236	10.744 8.407	32.987	47.035 47.781	1.00 16.65 1.00 16.37	B	c
	ATOM	2947	0		B 236	9.274	28.460	47.824	1.00 15.52	В	ŏ
55	ATOM	2949	N	THR	B 237	7.138	29.086	48.109	1.00 17.75	В	N
	ATOM	2950	CA	THR	B 237	6.685	27.770	48.545	1.00 18.73	В	C
	ATOM	2951	CB		в 237	5.203	27.813	49.028	1.00 20.81	B	C
	ATOM	2952	OG1 CG2		B 237 B 237	5.124 4.677	28.585 26.420	50.224 49.334	1.00 20.67 1.00 20.82	В	C
60	ATOM	2953 2954	C		B 237	6.818	26.764	47.410	1.00 18.80	В	č
00	ATOM	2955	ŏ		B 237	7.425	25.710	47.576	1.00 20.21	В	0
	ATOM	2956	N	GLU	B 238	6.253	27.092	46.252	1.00 20.60	В	N
	ATOM	2957	CA		B 238	6.320	26.199	45.099	1.00 19.19	В	C
65	MOTA	2958	CB		B 238 B 238	5.555 4.036	26.813 26.779	43.918 44.100	1.00 20.66 1.00 23.37	B	C
03	MOTA	2959 2960	CD		B 238	3.313	27.786	44.100	1.00 24.80	В	č
	ATOM	2961			B 238	3.581	27.842	42.009	1.00 25.78	В	0
	ATOM	2962	OE2	GLU	в 238	2.466	28.527	43.755	1.00 28.41	В	0
	ATOM	2963	C		В 238	7.767	25.917	44.705	1.00 19.31	В	C
70	ATOM	2964 2965	N		B 238 B 239	8.126 8.598	24.780 26.954	44.361 44.751	1.00 17.16 1.00 18.37	B B	O
	ATOM	2965	CA		B 239	10.004	26.801	44.401	1.00 17.98	В	c

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		ATOM	2967	CB		B 239	10.690		44.357	1.00 19.30	В	С
		ATOM	2968	CG		в 239	10.569		43.002	1.00 22.62	В	C
		ATOM	2969			в 239	10.915		43.126	1.00 23.53	В	C
	5	ATOM	2970			B 239	11.493	28.157	42.008	1.00 23.78	В	C
	J	ATOM	2971 2972	C	LEU	B 239 B 239	10.746 11.517	25.877 25.025	45.362 44.926	1.00 18.38	B B	0
		ATOM	2973	N	AT.A	B 240	10.514	26.047	46.665	1.00 16.60	В	N
		MOTA	2974	CA		B 240	11.180		47.668	1.00 17.68	В	Ĉ
		ATOM	2975	CB		B 240	10.830		49.080	1.00 16.34	В	č
	10	ATOM	2976	С	ALA	B 240	10.777	23.750	47.496	1.00 18.39	В	C
		ATOM	2977	0		B 240	11.606		47.641	1.00 16.04	В	0
		MOTA	2978	N		B 241	9.502	23.518	47.179	1.00 19.07	В	N
		ATOM	2979	CV		B 241	9.009	22.166	46.967	1.00 21.46	В	c
	15	ATOM ATOM	2980 2981	CB		B 241 B 241	7.517 6.625	22.167 22.096	46.602 47.814	1.00 23.76 1.00 28.59	В	C
	13	ATOM	2982			B 241	6.917	21.367	48.759	1.00 28.59	В	0
		ATOM	2983			B 241	5.524		47.794	1.00 29.40	В	N
		ATOM	2984	С		B 241	9.789		45.833	1.00 21.94	В	,c
		ATOM	2985	0		B 241	10.282	20.408	45.951	1.00 23.36	В	o
- 1	20	ATOM	2986	N		B 242	9.898		44.735	1.00 20.78	В	N
		ATOM	2987	CA		B 242	10.614		43.553	1.00 21.85	В	C
		ATOM ATOM	2988 2989	CB	ALA	B 242	10.437 12.105	22.818	42.426	1.00 18.99	В	C C
		ATOM	2990	ŏ	ALA		12.634		43.820 43.488	1.00 21.42 1.00 21.59	B	Ö
	25	ATOM	2991	N	LEU		12.782		44.426	1.00 22.94	В	N
		ATOM	2992	CA	LEU		14.209		44.730	1.00 21.96	В	č
		ATOM	2993	CB	LEU		14.751	23.669	45.360	1.00 19.53	В	C
		ATOM	2994	CG	LEU		14.744		44.439	1.00 20.66	В	C
		ATOM	2995		LEU		15.174		45.213	1.00 20.26	В	C
	30	ATOM	2996 2997			B 243 B 243	15.674		43.266	1.00 20.88 1.00 21.93	В	C
		ATOM	2998	c		B 243 B 243	14.457 15.449	21.196	45.668 45.535	1.00 21.93 1.00 20.07	B B	C
		ATOM	2999	N		B 244	13.558		46.626	1.00 22.84	В	N
		ATOM	3000	CA		B 244	13.676		47.572	1.00 25.72	В	č
	35	ATOM	3001	CB	SER		12.528	19.966	48.582	1.00 26.38	В	C
		ATOM	3002	OG	SER		12,707	18.992	49.589	1.00 31.74	В	0
		MOTA	3003	С	SER		13.646	18.594	46.800	1.00 26.65	В	C
		ATOM	3004	0		B 244	14.497	17.725	47.001	1.00 28.75	В	0
	40	MOTA MOTA	3005 3006	N CA	TYR	B 245 B 245	12.667 12.545	18.450 17.246	45.912 45.101	1.00 25.41 1.00 26.59	В	N C
	70	ATOM	3007	CB		B 245	11.297	17.347	44.210	1.00 28.39	В	č
		ATOM	3008	CG		B 245	11.234		43.050	1.00 29.48	В	č
		ATOM	3009	CD1	TYR	B 245	11.789	16.695	41.808	1.00 27.01	В	C
		ATOM	3010	CE1		B 245	11.746	15.806	40.740	1.00 25.91	В	C
	45	ATOM	3011	CD2	TYR		10.625	15.113	43.193	1.00 29.43	В	C
		ATOM ATOM	3012 3013	CE2	TYR		10.576 11.144		42.124	1.00 29.19 1.00 27.94	B	C
		ATOM	3014	OH	TYR		11.131	13.687	39.842	1.00 26.95	В	ŏ
		ATOM	3015	c	TYR		13.808	17.026	44.261	1.00 27.59	В	č
	50	MOTA	3016	0	TYR	B 245	14.272	15.897	44.117	1.00 27.11	В	ō
		ATOM	3017	N	CYS		14.372	18.099	43.711	1.00 27.30	В	N
		ATOM	3018	CA	CYS		15.586	17.965	42.907	1.00 27.67	В	c
		ATOM ATOM	3019 3020	CB	CYS		15.926 14.898	19.284 19.706	42.202 40.755	1.00 27.42	B	C S
	55	ATOM	3021	c	CYS		16.787	17.518	43.753	1.00 26.99	В	c
		MOTA	3022	ŏ	CYS		17.568		43.333	1.00 24.30	В	ŏ
		ATOM	3023	N	HIS		16.938		44.940	1.00 27.86	В	N
		MOTA	3024	CA		B 247	18.048	17.734	45.813	1.00 28.63	В	C
		MOTA	3025	CB	HIS		18.007	18.546	47.116	1.00 27.63	В	C
	60	MOTA	3026	CG	HIS		18.519	19.950	46.976	1.00 27.06	В	C
		MOTA MOTA	3027 3028		HIS	B 247 B 247	18.746 18.873	20.716	45.882 48.062	1.00 26.78 1.00 26.58	B	C N
		MOTA	3029		HIS		19.299	21.902	47.643	1.00 24.28	В	C
		MOTA	3030			B 247	19.232	21.923	46.325	1.00 24.21	В	N
	65	MOTA	3031	С	HIS	B 247	18.006	16.241	46.128	1.00 30.30	В	C
		MOTA	3032	0		B 247	19.046	15.594	46.243	1.00 29.75	В	0
		MOTA	3033	N	SER		16.801	15.691	46.245	1.00 31.77	В	N
		ATOM	3034 3035	CA	SER		16.641	14.275	46.550	1.00 34.48	В	C
	70	ATOM	3035	CB OG	SER		15.169 14.419	13.943 13.874	46.824 45.621	1.00 34.54 1.00 34.42	B	0
		ATOM	3037	C		B 248			45.417	1.00 36.24	В	c
		ATOM	3038	ŏ		B 248		12.239	45.640	1.00 39.13	В	ŏ
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							-87-				
	ATOM	3039	N	LYS	B 249	17.206		44.205	1.00 37.4	19 1	3 N
	ATOM	3040	CA	LYS	B 249	17.714		43.065	1.00 38.3		
	ATOM	3041	CB	LYS		16.752	13.291	41.882	1.00 39.5		
5	ATOM	3042	CG	LYS		15.480	12.470	42.075	1.00 41.0	9 1	з с
,	ATOM ATOM	3043 3044	CD	LYS		14.692	12.348	40.783	1.00 42.8		3 C
	ATOM	3044	NZ		B 249 B 249	13.544	11.345	40.903	1.00 44.6		
	ATOM	3046	C		B 249	14.008 19.110	9.940 13.649	41.115	1.00 43.8		
	ATOM	3047	ŏ		B 249	19.535	13.500	42.507	1.00 38.2		
10	ATOM	3048	N		B 250	19.823	14.208	43.639	1.00 38.1		
	ATOM	3049	CA	ALA	B 250	21.180	14.693	43.429	1.00 38.8		
	ATOM	3050	CB	ALA	B 250	22.128	13.506	43.260	1.00 37.3		
	ATOM	3051	C		B 250	21.294	15.642	42.234	1.00 39.6		
15	ATOM	3052	0		B 250	22.256	15.586	41.469	1.00 39.7		3 0
13	ATOM	3053 3054	N CA		B 251 B 251	20.312	16.521	42.077	1.00 40.6		
	ATOM	3055	CB		B 251	20.331 19.009	17.475 17.448	40.976	1.00 41.4		
	ATOM	3056			B 251	18.996	18.543	40.197 39.156	1.00 39.7		
	ATOM	3057		VAL		18.833	16.099	39.542	1.00 36.9		
20	ATOM	3058	С	VAL	B 251	20.575	18.887	41.487	1.00 43.3		
	ATOM	3059	0	VAL		19.857	19.361	42.361	1.00 43.1		
	ATOM	3060	N	ALA		21.594	19.572	41.411	1.00 47.2		
	MOTA	3061	CA		B 252	21.800	20.930	41.937	1.00 51.5		c
25	ATOM	3062 3063	CB	ALA		23.072	20.979	42.781	1.00 50.0		
23	ATOM	3064	C	ALA		21.867 22.516	21.974	40.811	1.00 55.1		
	ATOM	3065	N	HIS		21.201	23.110	39.786 41.025	1.00 55.3 1.00 59.2		
	ATOM	3066	CA	HIS		21.127	24.196	40.039	1.00 59.2		
	ATOM	3067	CB	HIS		19.928	25.100	40.346	1.00 63.3		
30	ATOM	3068	CG		B 253	18.626	24.569	39.838	1.00 65.5	8 B	
	ATOM	3069		HIS		17.728	25.093	38.970	1.00 65.7	8 B	č
	ATOM	3070			B 253	18.131	23.335	40.205	1.00 66.2	1 в	N
	ATOM	3071 3072			B 253 B 253	16.985	23.122	39.583	1.00 66.2		
35	ATOM	3072	C		B 253	16.718 22.343	24.173	38.828	1.00 66.3		
	ATOM	3074	ŏ	HIS		23.157	25.091 24.827	39.812 38.924	1.00 64.2		
	ATOM	3075	N	ARG		22.431	26.162	40.603	1.00 66.2		
	ATOM	3076	CA	ARG		23.501	27.162	40.503	1.00 67.9		
40	MOTA	3077	CB	ARG	B 254	24.829	26.507	40.106	1.00 69.3		
40	ATOM	3078	CG	ARG		25.429	25.629	41.199	1.00 72.1	в в	č
	ATOM	3079 3080	CD NE	ARG	B 254	26.435	24.626	40.649	1.00 73.8		C
	ATOM	3081	CZ	ARG	B 254 B 254	27.423 28.423	25.232 24.559	39.760	1.00 76.1		N
	ATOM	3082		ARG	B 254	28.566	23.259	39.197 39.435	1.00 77.33		С
45	ATOM	3083	NH2	ARG	B 254	29.275	25.180	38.391	1.00 77.4		N
	MOTA	3084	С	ARG	B 254	23.093	28,203	39.455	1.00 68.10		c
	ATOM	3085	0		B 254	23.941	28.818	38.805	1.00 68.48		ŏ
	ATOM	3086	N		B 255	21.779	28.383	39.311	1.00 67.9	1 в	N
50	ATOM	3087 3088	CB		B 255	21.181	29.321	38.358	1.00 66.09		С
30	ATOM	3089	CG		B 255 B 255	21.768 20.978	29.117 29.848	36.960	1.00 68.18		C
	ATOM	3090	OD1		B 255	20.978	31.098	35.891 35.906	1.00 70.20		c
	ATOM	3091			B 255	20.346	29.176	35.045	1.00 70.61		0
	ATOM	3092	C	ASP	B 255	19.670	29.086	38.290	1.00 64.02		c
55	MOTA	3093	0		B 255	19.224	27.980	37.966	1.00 63.85		ŏ
	ATOM	3094	N		B 256	18.887	30.123	38.587	1.00 60.24	В	N
	ATOM	3095 3096	CA		B 256	17.432	30.007	38.557	1.00 56.06		c
	ATOM	3096	CB CG2		B 256 B 256	16.938	29.251	39.813	1.00 56.48		C
60	ATOM	3098	CG1		B 256	17.097 15.483	30.123 28.833	41.051 39.637	1.00 57.30		c
	ATOM	3099	CD1		B 256	15.012	27.833	40.671	1.00 56.77		c
	ATOM	3100	С	ILE		16.727	31.371	38.444	1.00 52.46		c
	ATOM	3101	0	TLE :	B 256	15.769	31.661	39.154	1.00 51.61		ŏ
ce	ATOM	3102	N		в 257	17.209	32.193	37.521	1.00 48.41		N
65	MOTA	3103	CA		B 257	16.684	33.536	37.258	1.00 44.89	В	c
	ATOM ATOM	3104 3105	CB		B 257 B 257	17.469	34.142	36.094	1.00 45.52		c
	ATOM	3105	CD		B 257	18.981 19.703	34.051	36.249	1.00 48.52		c
	ATOM	3107	CE		B 257	19.703	34.586 33.695	35.017 33.791	1.00 50.54		c
70	ATOM	3108	NZ		B 257	20.251	32.406	33.875	1.00 50.70	В	C N
	ATOM	3109	C		B 257	15.177	33.614	36.941	1.00 40.75		C
	ATOM	3110	0	LYS :	B 257	14.548	32.614	36.614	1.00 40.52	В	ŏ

							-88-						
	ATOM	3111	N	PRO B	258	14.480	34.397	36.931	1.00	37.08	1	3 1	N
	ATOM	3112	CD	PRO B		15.445	35.391	37.431		36.34			С
	ATOM	3113	CA	PRO B		13.167	35.015	36.690		35.17			c
5	MOTA MOTA	3114	CB	PRO B		13.397 14.544	36.489 36.448	37.038 38.017		34.26			c
,	ATOM	3116	C	PRO B		12.770	34.825	35.227		34.61			c
	MOTA	3117	ō	PRO B		11.604	34.576	34.908	1.00	31.39			ō
	MOTA	3118	N	GLU B		13.757	34.954	34.346	1.00	33.54			N
	MOTA	3119	CA	GLU B		13.540	34.769	32.918		34.62			С
10	MOTA	3120	CB	GLU B		14.706 15.143	35.332 36.745	32.100 32.442		37.22 41.67		B (C
	ATOM ATOM	3121 3122	CD	GLU B		15.934	36.826	33.735		44.39			c
	MOTA	3123	OE1			16.564	37.874	33.978		46.55			ō
	ATOM	3124	OE2	GLU B		15.924	35.851	34.515		46.90			0
15	MOTA	3125	c	GLU B		13.469	33.265	32.678		34.06			c
	ATOM	3126	0		259 260	13.004 13.943	32.812 32.492	31.632 33.652		34.68			N
	ATOM	3127 3128	N CA	ASN B		13.941	31.042	33.527		30.54			C
	ATOM	3129	CB	ASN B		15.262	30.455	34.035		34.15			č
20	ATOM	3130	CG	ASN B		16.474	31.178	33.478		39.70			С
	ATOM	3131		ASN B		16.454	31.681	32.347		41.30			0
	ATOM	3132		ASN B		17.545	31.226	34.265		40.33			N C
	ATOM	3133 3134	C	ASN B		12.785 12.723	30.413 29.194	34.284		27.70			0
25	ATOM	3135	N	LEU B		11.879	31.244	34.783		23.87			N
	ATOM	3136	CA	LEU B		10.715	30.748	35.511	1.00	23.63			С
	MOTA	3137	CB	LEU B		10.636	31.393	36.904		23.52			С
	ATOM	3138	CG	LEU B		11.859 11.784	31.157 32.065	37.802 39.013	1.00	23.80		В	c
30	MOTA	3139 3140		LEU B		11.784	29.696	38.233		23.15			c
50	ATOM	3141	c	LEU B		9.486	31.094	34.683		22.79		В	c
	ATOM	3142	ō	LEU B		9.248	32.259	34.360	1.00	23.35		в	0
	MOTA	3143	N	LEU B		8.720	30.072	34.329		21.85			N
35	MOTA	3144 3145	CA	LEU B		7.530 7.583	30.240 29.241	33.503 32.338		20.81			c
33	MOTA	3145	CB	LEU B		8.805	29.241	31.427		20.74		В	č
	ATOM	3147		LEU B		9.022	28.247	30.528		17.18			č
	MOTA	3148		LEU B		8.594	30.704	30.600		23.22			С
	ATOM	3149	С	LEU B		6.260	30.050	34.324		20.95			c
40	MOTA	3150 3151	O	LEU B		6.320 5.118	29.607 30.385	35.468 33.731		21.65			O N
	ATOM	3152	CA	LEU B		3.818	30.291	34.401	1.00	19.89			Č
	MOTA	3153	CB	LEU B		3.199	31.682	34.542	1.00	19.96			С
	MOTA	3154	CG	LEU B		3.895	32.673	35.485		22.61			С
45	MOTA	3155		LEU B		3.332	34.074	35.269		19.88		В	c
	ATOM	3156 3157	CD2	LEU B		3.689 2.828	32.218 29.405	36.938 33.667		19.42			c
	MOTA	3158	ŏ	LEU B		2.555	29.607	32.477		19.05			ŏ
	ATOM	3159	N	GLY B	264	2.285	28.434	34.390	1.00	20.39			N
50	MOTA	3160	CA	CTA B		1.318	27.531	33.810		22.81			С
	MOTA	3161 3162	C	GLY B		-0.058 -0.267	28.166 29.307	33.723 34.146		23.93			c o
	ATOM	3163	И	SER B		-0.996	27.406	33.178		26.43			N
	ATOM	3164	CA	SER B	265	-2.375	27.846	33.002		29.74		в	С
55	MOTA	3165	CB	SER B		-3.224	26.687	32.478		30.89			С
	MOTA	3166	OG	SER B		-4.593	27.054	32.458		37.32			0
	ATOM	3167 3168	c	SER B		-3.026 -3.786	28.398 29.356	34.267		30.10			C
	ATOM	3169	N	ALA B		-2.738	27.790	35.411		29.46			N
60	MOTA	3170	CA	ALA B		-3.319	28.239	36.670	1.00	28.49		в	С
	MOTA	3171	CB	ALA B		-3.645	27.040	37.546		27.90			C
	ATOM	3172	C	ALA B		-2.424	29.202	37.433		27.49			C
	MOTA	3173 3174	N O	ALA B GLY B		-2.673 -1.380	29.486 29.704	38.594 36.785		26.71 28.52			N O
65	ATOM	3175	CA	GLY B		-0.485	30.630	37.458		27.29			c
	MOTA	3176	C	GLY B	267	0.556	29.951	38.335	1.00	26.61		в	С
	MOTA	3177	0	CLY B		1.155	30.591	39.203		27.45			0
	MOTA	3178	N	GLU B		0.780	28.660	38.117		25.29			N
70	MOTA	3179 3180	CB	GLU B		1.766	27.924	38.905 38.967		26.30 27.43			c
,0	ATOM	3181	CG	GLU B		0.012	26.107	38.488		34.47			c
	ATOM	3182	CD	GLU B		-0.087	26.008	36.976		35.53			c

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	MOTA	3183		GLU		0.297	24.958	36.423	1.00 38.92	В	0
	ATOM	3184	OE2		B 268	-0.546	26.979	36.339	1.00 38.49	В	0
	ATOM	3185 3186	C		B 268 B 268	3.154	28.083	38.287	1.00 24.38	В	C
5	ATOM	3187	N	CLU	B 268	3.300 4.171	28.062 28.250	37.063 39.129	1.00 21.68 1.00 23.82	B B	0
,	ATOM	3188	CA	PEO	B 269	5.542	28.398	38.634	1.00 23.82	В	N C
	ATOM	3189	CB		B 269	6.492	28.808	39.761	1.00 24.33	В	č
	ATOM	3190	CG	LEU	B 269	6.545	30.246	40.265	1.00 25.70	В	c
	ATOM	3191		LEU		7.693	30.382	41.252	1.00 24.92	В	C
10	ATOM .	3192		LEU		6.751	31.198	39.103	1.00 27.39	В	C
	MOTA	3193	C		B 269	6.061	27.099	38.034	1.00 19.77	В	C
	ATOM ATOM	3194 3195	0		B 269 B 270	5.703	26.015	38.485	1.00 19.34	В	0
	ATOM	3195	N CA		B 270	6.909 7.525	27.222 26.074	37.017 36.356	1.00 19.92 1.00 20.30	B B	N
15	ATOM	3197	CB		B 270	6.902	25.836	34.972	1.00 18.33	В	č
	ATOM	3198	CG		B 270	5.393	25.615	34.964	1.00 18.74	В	č
	ATOM	3199	CD		B 270	5.012	24.155	35.137	1.00 15.50	В	Ċ
	ATOM	3200	CE		B 270	3.491	23.994	35.128	1.00 18.10	В	C
20	ATOM	3201	NZ		B 270	3.046	22.575	35.077	1.00 15.24	В	N
20	MOTA	3202 3203	C		B 270 B 270	9.019 9.373	26.383	36.178	1.00 20.49	В	C
	ATOM	3203	0	ьть.	B 2/0	9.373	27.374	35.550	1.00 18.08	В	0
	MOTA	3204	N	ILE	B 271	9.889	25.545	36.737	1.00 21.09	В	N
	MOTA	3205	CA		B 271	11.329	25.756	36.587	1.00 20.68	В	C
25	MOTA	3206	CB		B 271	12.133	25.016	37.674	1.00 21.21	В	С
	ATOM ATOM	3207 3208	CG2	ILE	B 271	13.640	25.176	37.413	1.00 19.34	В	C
	ATOM	3208		ILE		11.761 12.514	25.553 24.863	39.060 40.210	1.00 23.24 1.00 24.09	B B	C
	ATOM	3210	C		B 271	11.754	25.207	35.224	1.00 20.59	В	c
30	ATOM	3211	ō		B 271	11.482	24.051	34.911	1.00 19.44	B	ŏ
	ATOM	3212	N	ALA:	B 272	12.410	26.034	34.416	1.00 19.34	В	N
	ATOM	3213	CA		B 272	12.858	25.598	33.095	1.00 24.16	В	C
	ATOM ATOM	3214 3215	CB		B 272 B 272	12.404	26.594	32.037	1.00 20.99	В	Ċ
35	ATOM	3215	C		B 272	14.384 15.106	25.434 26.155	33.039 33.723	1.00 26.77 1.00 27.46	B B	C
	ATOM	3217	N		B 273	14.843	24.478	32.225	1.00 29.94	В	N
	ATOM	3218	CA	ASP		16.265	24.150	32.014	1.00 32.45	В	c
	MOTA	3219	CB		B 273	17.153	25.351	32.319	1.00 33.94	В	C
40	ATOM	3220	CG		B 273	17.622	26.038	31.068	1.00 38.34	В	C
40	MOTA	3221		ASP		18.171	27.165	31.162	1.00 41.51	В	0
	ATOM	3222 3223	C C	ASP :		17.439 16.799	25.436 22.930	29.986 32.767	1.00 36.50 1.00 34.27	B B	0
	ATOM	3224	ŏ	ASP		17.928	22.472	32.518	1.00 34.27	В	Ö
	ATOM	3225	N	GLY		22.452	32.822	36.840	1.00 57.41	В	N
45	ATOM	3226	CA	GLY :	B 290	22.919	33.188	35.513	1.00 56.55	В	c
	ATOM	3227	C	GLY :		23.992	34.260	35.563	1.00 56.09	В	C
	ATOM	3228	0	GLY :		25.185	33.954	35.650	1.00 56.35	В	0
	ATOM	3229 3230	N CA	THR :		23.572 24.511	35.522 36.633	35.508 35.555	1.00 54.56 1.00 52.44	В	N
50	ATOM	3231	CB	THR		23.813	37.967	35.195	1.00 52.44	B	C
-	ATOM	3232		THR		22.687	38.172	36.056	1.00 54.88	В	ŏ
	ATOM	3233	CG2	THR :		23.338	37.946	33.746	1.00 55.03	В	č
	ATOM	3234	C	THR :		25.140	36.738	36.945	1.00 50.11	B	C
	ATOM	3235	0	THR		24.840	35.940	37.840	1.00 47.96	В	0
55	ATOM	3236 3237	N CA	PEA :	B 292	26.010 26.695	37.727	37.123	1.00 47.85	B	N
	ATOM	3238	CB	LEU :		27.664	37.926 39.109	38.395 38.280	1.00 46.13 1.00 46.70	В	C
	ATOM	3239	CG		3 292	28.706	39.250	39.393	1.00 47.14	В	č
	ATOM	3240			3 292	29.422	37.921	39.596	1.00 46.68	В	č
60	MOTA	3241	CD2		B 292	29.704	40.342	39.030	1.00 46.77	В	C
	MOTA	3242	C		3 292	25.740	38.143	39.573	1.00 44.02	В	C
	ATOM	3243 3244	O		3 292 3 293	25.967	37.638	40.675	1.00 43.84	В	0
	ATOM	3244	CA		3 293	24.663 23.687	38.879 39.172	39.330 40.371	1.00 41.14	B	N
65	ATOM	3246	CB		3 293	22.551	40.010	39.789	1.00 40.18	В	C
	ATOM	3247	CG		3 293	22.969	41.428	39.508	1.00 39.93	В	c
	MOTA	3248		ASP I	3 293	23.770	41.635	38.578	1.00 43.70	В	ō
	ATOM	3249		ASP I		22.510	42.336	40.227	1.00 42.04	В	0
70	MOTA	3250 3251	C		3 293	23.084	37.986	41.124	1.00 38.77	В	C
/0	ATOM	3251	N		3 293 3 294	22.442 23.288	38.175 36.770	42.157 40.628	1.00 36.99 1.00 38.33	B	O
	ATOM	3253	CA		3 294	22.704	35.607	41.284	1.00 36.46	В	C

							00					
	ATOM	3254	СВ	TYR E	204	21.721	-90- 34.923	40.324	1 00	37.01	Е	c
	ATOM	3255	CG	TYR E		20.645	35.862	39.813		36.29	P	
	ATOM	3256	CD1	TYR E		20.894	36.732	38.747		36.77	Ē	
	ATOM	3257	CE1	TYR E		19.932	37.650	38.324	1.00	35.17	E	
5	ATOM	3258	CD2	TYR E		19.405	35.931	40.440		33.86	E	
	ATOM	3259	CE2	TYR E		18.438	36.841	40.029		34.67	В	
	ATOM	3260	OH	TYR E		18.707	37.700	38.974		36.81	Е	
	ATOM	3261 3262	C	TYR E		17.747 23.674	38.614 34.573	38.586 41.855		37.64	E E	
10	ATOM	3263	ö	TYR E		23.241	33.612	42.482		33.83	E	
	ATOM	3264	N	LEU B		24.975	34.768	41.664	1.00	34.16	E	
	ATOM	3265	CA	LEU B	295	25.946	33.804	42.180	1.00	34.73	E	
	ATOM	3266	CB	PEA B		27.191	33.790	41.287	1.00	35.44	В	C
	ATOM	3267	CG	LEU B		26.941	33.402	39.822		37.31	В	
15	ATOM	3268	CD1	PEA B		28.232	33.537	39.015		38.09	Е	
	MOTA MOTA	3269 3270	CD2	PER B		26.409 26.340	31.974 34.071	39.754 43.635		37.09	E E	
	ATOM	3271	ò	PEA B		26.485	35.220	44.045		33.23	E	
	ATOM	3272	N	PRO B		26.501	33.003	44.438		32.82	B	
20	ATOM	3273	CD	PRO B		26,174	31.603	44.099		32.14	В	
	MOTA	3274	CA	PRO B		26.877	33.123	45.852	1.00	32.58	В	C
	ATOM	3275	CB	PRO B		26.408	31.796	46.442		30.74	В	
	ATOM	3276	CG	PRO B		26.654	30.841	45.321		30.81	В	
25	MOTA MOTA	3277 3278	C	PRO B		28.380 29.185	33.355 33.190	46.069 45.150		34.00	В	
23	ATOM	3279	N	PRO E		28.771	33.744	47.297		35.08	B	
	ATOM	3280	CD	PRO E		27.894	34.068	48.438		34.25	В	
	MOTA	3281	CA	PRO B		30.174	33.999	47.639		36.33	3	
	MOTA	3282	CB	PRO B		30.111	34.293	49.137		34.76	В	C
30	MOTA	3283	CG	PRO B		28.777	34.948	49.287		34.10	В	
	MOTA	3284	C	PRO B		31.128	32.840	47.314		37.57	В	
	ATOM ATOM	3285 3286	O N	PRO B		32.097	33.021	46.583		39.23	В	
	ATOM	3287	CA	GLU B		30.847	31.654 30.491	47.848 47.626		38.80 40.63	B	
35	ATOM	3288	CB	GLU B		31.108	29.232	48.260		39.54	В	
	ATOM	3289	CG	GLU B		29.823	28.761	47.590	1.00	38.57	В	
	ATOM	3290	CD	GLU B		28.592	29.251	48.313	1.00	37.66	В	C
	ATOM	3291	OE1	GLU B		28.601	30.406	48.795		38.14	В	
40	ATOM ATOM	3292 3293	OE2	GLU B		27.618	28.481	48.400		36.41	В	
40	ATOM	3293	C	GLU B		32.016 32.873	30.187 29.355	46.164 45.874		42.36	B B	CO
	ATOM	3295	N	MET B		31.317	30.837	45.241		44.46	В	
	ATOM	3296	CA	MET B		31.572	30.589	43,830	1.00	46.93	В	
	ATOM	3297	CB	MET B		30.262	30.454	43.054		47.22	В	
45	ATOM	3298	CG	MET B		29.494	29.190	43.410		49.38	В	
	ATOM	3299 3300	SD	MET B		28.411	28.637	42.093	1.00		В	
	ATOM	3301	C	MET B		29.502 32.447	27.513 31.662	41.247		53.08 47.79	B	C
	ATOM	3302	ò	MET B		33.416	31.350	42.522		48.57	В	
50	ATOM	3303	N	ILE B		32.118	32.926	43.457		48.73	В	
	ATOM	3304	CA	ILE B		32.930	34.004	42.914	1.00	49.57	В	C
	ATOM	3305	CB	ILE B		32.190	35.362	42.968	1.00	49.76	В	
	ATOM	3306	CG2	ILE B		30.896	35.273	42.171		49.66	В	
55	MOTA	3307 3308	CG1	ILE B		31.904	35.761 37.143	44.416		48.39 47.07	В	C
55	ATOM	3309	CDI	ILE B		34.243	34.096	43.697		50.74	В	c
	ATOM	3310	ŏ	ILE B		35.253	34.571	43.177		50.30	В	ŏ
	MOTA	3311	N	GLU B	301	34.226	33.630	44.943		52.24	В	N
	MOTA	3312	CA	GLU B		35.424	33.648	45.776		54.57	В	C
60	ATOM	3313	CB	GLU B		35.058	33.596	47.267	1.00		В	C
	MOTA	3314 3315	CD	GLU B		34.210	34.770	47.737	1.00	58.62	В	c
	ATOM	3316	OE1	GLU B		34.020 33.827	34.806 33.731	49.247 49.855	1.00	59.50 60.80	B	C
	ATOM	3317	OE2	GLU B		34.046	35.915	49.823		59.81	B	0
65	ATOM	3318	C	GLU B		36.309	32.456	45.421		55.44	В	č
	ATOM	3319	o	GLU B	301	37.419	32.322	45.936	1.00	55.50	В	ō
	ATOM	3320	N	GLY B		35.804	31.590	44.544	1.00	55.63	В	N
	ATOM ATOM	3321	CA	GLY B		36.567	30.429	44.119		56.55	В	C
70	ATOM	3322 3323	C	GLY B		36.457 36.823	29.193 28.100	44.995		57.16 57.49	B	C
,,,	ATOM	3324	N	ARG B		35.966	29.359	46.221	1.00		В	И
	ATOM	3325	CA	ARG B		35.808	28.241	47.149	1.00		В	Č
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	ATOM	3326	СВ	ARG	В	3.03	35.094	28.702	48.419	1.00	58.72	В	С
	ATOM	3327	CG	ARG			35.855	29.706	49.257	1.00	61.00	в	C
	ATOM	3328	CD	ARG	В	303	34.963	30.239	50.366	1.00	62.94	В	C
	MOTA	3329	NE	ARG		303	35.680	31.094	51.309	1.00	64.60	В	N
5	ATOM	3330	CZ	ARG		303	36.606	30.661	52.160	1.00	65.49 65.70	B B	C
	ATOM	3331		ARG		303	37.203 36.936	31.514 29.376	52.982 52.191	1.00	65.53	В	N
	ATOM	3332 3333	NH2 C	ARG		303	34.995	27.119	46.517	1.00		В	c
	ATOM	3334	ò	ARG		303	34.586	27.209	45.358	1.00	58.81	В	o
10	ATOM	3335	N	MET		304	34.758	26.060	47.284	1.00	57.39	В	N
	ATOM	3336	CA	MET	В	304	33.974	24.934	46.792		56.99	В	С
	MOTA	3337	CB			304	34.389	23.647	47.508		59.63	в	C
	MOTA	3338	CG		В	304	34.471	22.435	46.594		63.14	В	c
	ATOM	3339	SD		В	304	32.911	22.046	45.769 46.851		67.12	В	c
15	MOTA	3340	CE		В	304	32.278 32.504	25.247	47.072		54.74	В	č
	ATOM	3341 3342	0		В	304	32.197	26.264			53.70	В	ŏ
	ATOM	3343	N		В	305	31.600			1.00	52.40	В	N
	ATOM	3344	CA		В	305	30.170	24.598	46.826		49.37	В	C
20	MOTA	3345	CB	HIS	В	305	29.638		45.791		49.86	в	C
	MOTA	3346	CG	HIS	В	305	29.857	25.138			51.90	В	C
	ATOM	3347			В	305	28.986				52.04 51.78	В	N
	ATOM	3348	ND1		В	305 305	31.110 31.000				53.53	В	C
25	ATOM	3349 3350	NE2				29.723	24.395			53.06	В	N
23	ATOM	3351	C	HIS			29.347	23.312		1.00	46.97	в	C
	ATOM	3352	ŏ			305	29.791			1.00	46.30	в	0
	ATOM	3353	N			306	28.135				43.16	В	N
	ATOM	3354	CA			306	27.246				40.92	В	C
30	MOTA	3355	CB			306	27.405				40.71	В	C
	ATOM	3356	CG	ASP	В	306	26.952 26.828				40.70	В	ŏ
	MOTA	3357 3358	ODI	ASP	B	306	26.729				42.16	В	ŏ
	ATOM	3359	C	ASP	В	306	25.797	22.670			39.86	В	C
35	ATOM	3360	ŏ			306	25.545	23.734	46.505	1.00	39.27	В	0
	ATOM	3361	N			307	24.851	. 21.858	47.542		37.39	В	N
	ATOM	3362	CA			307	23.437	22.179	47.392		35.90	В	C
	ATOM	3363	CB			307	22.562		47.939 48.370		37.19 42.69	В	c
40	MOTA	3364 3365	CD			307 307	23.310 23.978	19.79	49.723		43.86	В	č
40	ATOM	3366		GLU			23.275	20.24			46.08	В	ō
	ATOM	3367		GLU			25.205	19.74	49.798		45.78	В	0
	MOTA	3368	C	GLU	В	307	23.049	23.48	48.083		34.05	В	C
	ATOM	3369	0			307	21.948	24.00	47.862		30.38	В	0
45	ATOM	3370	N			308	23.953	24.01			29.97 27.77	В	N
	ATOM	3371	CA			308	23.660				29.00	В	č
	ATOM	3372 3373	CG			308	24.669			1.00	30.48	В	č
	ATOM	3374	CD			308	23.346			1.00	31.68	В	С
50		3375	CE	LYS	В	308	23.442	23.78	3 53.921		32.64	В	C
	ATOM	3376	NZ			308	22.194				32.70	В	N
	MOTA	3377	С	LYS	В	308	23.536				25.47	В	C
	MOTA	3378	0	LYS	В	308	23.00				23.68	В	N
55	ATOM	3379 3380	N CA			309	23.894				23.94	B	Ĉ
33	ATOM	3381	CB	VAI.	·P	309	24.66				23.56	В	C
	ATOM	3382		. VAL	E	309	26.14		5 45.572	1.00	26.07	В	C
	ATOM	3383	CG2	VAL	E	309	24.10				23.94	В	С
	ATOM	3384	C			309	22.42				24.19	В	C
60	ATOM	3385	0			309	22.05		7 46.139		25.34	В	N O
	ATOM	3386	M.			310	21.58				22.68	В	C
	MOTA	3387 3388	CA			310	19.45				23.58	В	C
	ATOM	3389	CG	ASP			19.92				27.55	в	c
65	ATOM	3390				310	20.27		2 43.445	1.00	28.81	в	0
	ATOM	3391				310	19.93				31.31	В	0
	ATOM	3392	C	ASP			19.46				21.05	В	c
	ATOM	3393	0	ASE			18.51			1.00	20.77	В	14
70	MOTA MOTA	3394 3395	N CA	LEU		311	19.93 19.35			1.00	19.16	В	c
/0	MOTA	3395				3 3 1 1	19.88				19.21	В	С
	ATOM	3397	CG			3 311	19.20				21.60	В	C

							-92-	51.572	1.00 20.35	В	С
	MOTA	3398	CD1 I	EU B	311	17.737 19.360	27.054 25.484	50.528	1.00 19.65	В	C
	MOTA			EO B	311	19.664	29.934	49.174	1.00 19.50	В	С
	ATOM			EU B		18.853	30.791	49.530	1.00 17.78	В	0
	ATOM ATOM			RP B		20.848	30.245	48.653	1.00 20.26	B	N C
	ATOM			TRP B	312	21.226	31.634	48.452	1.00 19.28	В	c
	ATOM		CB S	TRP B	312	22.716	31.729	48.109	1.00 20.45 1.00 18.65	В	c
	MOTA	3405	CG S	TRP B	312	23.156	33.064	47.620 48.390	1.00 19.00	В	С
	ATOM	3406		TRP B	312	23.784	34.092 35.176	47.515	1.00 18.21	В	С
10	ATOM	3407		TRP B	312	24.161	34.205	49.733	1.00 20.36	В	С
	MOTA	3408		TRP B	312 312	23.048	33.551	46.344	1.00 20.44	В	C
	MOTA	3409 3410		TRP B	312	23.574	34.820	46.274	1.00 19.77	В	N
	ATOM	3411		TRP B	312	24.646	36.354	47.940	1.00 18.87	В	C
15	MOTA	3412		TRP B		24.771	35.379	50.157	1.00 19.61	В	č
IJ	ATOM	3413		TRP B		25.007	36.438	49.260	1.00 21.25 1.00 20.24	В	č
	ATOM	3414	С	TRP B		20.389	32.206	47.326	1.00 18.37	В	ō
	ATOM	3415	0	TRP B		19.903	33.334	47.408 46.263	1.00 20.08	В	N
	ATOM	3416		SER B		20.236	31.421	45.113	1.00 19.43	В	C
20	ATOM	3417		SER B		19.455 19.460	30.760	44.037	1.00 20.79	В	С
	MOTA	3418		SER E		20.741	30.657	43.448	1.00 24.62	В	0
	MOTA	3419		SER E		18.024	32.156	45.502	1.00 19.39	В	c
	MOTA	3420 3421	C	SER E		17.403	33.035	44.920	1.00 18.50	В	O N
25	MOTA MOTA	3422		LEU I		17.512	31.442	46.498	1.00 19.22	B B	C
25	ATOM	3423	CA	LEU I		16.141	31.641	46.960	1.00 19.58 1.00 20.69	В	č
	ATOM	3424	CB	LEU I		15.737	30.476	47.871	1.00 20.69	В	č
	ATOM	3425	CG	LEU I		14.276	30.024	47.987 46.608	1.00 20.26	В	c
	MOTA	3426	CD1	LEU I		13.682	29.761 28.758	48.843	1.00 20.22	В	С
30	ATOM	3427	CD2	PEO 1		14.215 16.021	32.976	47.693	1.00 19.00	В	C
	MOTA	3428	C	LEU I	B 314 B 314	14.973	33.637	47.632	1.00 20.65	В	0
	ATOM	3429	N	GLY I		17.097	33.372	48.375	1.00 17.95	В	N C
	ATOM	3430 3431	CA	GLY :		17.112	34.638	49.097	1.00 14.32	B B	c
35	ATOM	3432	c	GLY :		17.085	35.805	48.120	1.00 15.06	В	Ö
25	ATOM	3433	ŏ	GLY :	B 315	16.308	36.753	48.270	1.00 15.06 1.00 15.22	В	N
	ATOM	3434	N	VAL:	B 316	17.930	35.728	47.098 46.090	1.00 15.50	В	c
	ATOM	3435	CA	VAL		17.996	36.775	45.050	1.00 17.46	В	С
	MOTA	3436	CB	VAL		19.115	36.487 37.470	43.858	1.00 15.92	В	С
40		3437	CG1			19.005 20.492	36.626	45.715	1.00 15.82	В	C
	ATOM	3438	CG2	VAL		16.651	36.899	45.387	1.00 15.41	В	c
	ATOM	3439 3440	C	VAL		16.152	38.004	45.193	1.00 18.18	B B	O
	MOTA	3441	N	LEU		16.063	35.764	45.020	1.00 15.83	В	C
45		3442	CA	LEU		14.762	35.729	44.350		В	č
45	ATOM	3443	CB		B 317	14.399	34.276	44.019		В	č
	ATOM	3444	CG		B 317	14.200	33.825			В	C
	ATOM	3445			B 317	15.254 14.273				В	C
	MOTA	3446			B 317	13.653			1.00 17.12	В	С
50		3447			B 317 B 317	12.877			1.00 17.94	В	0
	ATOM	3448	0	CYS		13.575	35.961	46.472	1.00 15.77	В	N
	ATOM	3449 3450	CA	CYS		12.569		47.38	1.00 13.11	В	C
	ATOM ATOM	3451			B 318	12.718	35.837	48.76		B	s
5		3452		CYS	B 318	11.422				В	č
٥.	ATOM	3453		CYS	B 318	12.683	38.01			В	ō
	ATOM	3454			B 318	11.67				В	N
	ATOM	3455		TYR	B 319	13.91				В	C
	ATOM	3456		TYR		14.14: 15.64		7 47.99		В	C
6		345		TYR	B 319 B 319	16.02			1 1.00 18.67	В	C
	MOTA	345				16.10				В	C
	ATOM	345	9 CD	I TIK	B 313	201-1					С
	MOTA	346	O CE	1 TYR	в 319	16.46		8 47.17	2 1.00 22.71	B	C
6	5 ATOM					16.32			8 1.00 21.26	В	
0	ATOM ATOM				в 319	16.68				В	
	ATOM			TYR		16.75	2 44.38			В	
	ATOM	346	4 OH	TYR		17.07				В	C
	ATOM	346		TYP		13.71 13.00				В	. 0
7	MOTA 0			TYF		13.00			9 1.00 14.73	В	
	ATOM			GLU	рв 320 гв 320	13.78				В	C
	ATOM	340	o CA	, GDC	5.00						

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	ATOM	3469	CB	GLU :	в 320	14.463	40.031	42.853	1.00 17.46	В	C
	ATOM	3470	CG	GLU :		14.174	40.726	41.542	1.00 22.76	В	C
	MOTA	3471	CD	GLU I		15.125	40.341	40.423	1.00 26.48 1.00 28.28	B	0
	MOTA	3472	OE1	GLU :	в 320	15.023	40.974 39.426	39.359 40.592	1.00 26.25	В	ŏ
5	ATOM	3473		GLU :	B 320	15.967 12.264	40.748	43.811	1.00 17.10	В	c
	ATOM	3474 3475	C	GLU :	B 320 B 320	11.719	41.682	43.237	1.00 20.22	В	0
	ATOM ATOM	3475	N		B 321	11.573	39.720	44.276	1.00 17.49	В	N
	ATOM	3477	CA		B 321	10.126	39.703	44.121	1.00 18.22	В	C
10	ATOM	3478	CB	PHE		9.524	38.385	44.622	1.00 18.69	В	C
	ATOM	3479	CG	PHE	B 321	9.701	37.231	43.683	1.00 21.02	В	C
	ATOM	3480	CD1		B 321	10.056	37.439	42.351	1.00 21.40 1.00 22.14	В	c
	MOTA	3481	CD2		B 321	9.498	35.930 36,366	44.126 41.479	1.00 22.14	В	Ċ
	MOTA	3482	CE1		B 321	10.209 9.648	34.853	43.260	1.00 23.29	В	č
15	MOTA	3483 3484	CE2		B 321 B 321	10.006	35.073	41.935	1.00 22.08	В	С
	ATOM ATOM	3485	c		B 321	9.469	40.841	44.887	1.00 20.00	В	С
	ATOM	3486	ŏ		B 321	8.563	41.499	44.375	1.00 19.40	В	0
	ATOM	3487	N	LEU	B 322	9.919	41.057	46.123	1.00 20.34	В	N
20	ATOM	3488	CA		B 322	9.351	42.089	46.991	1.00 21.70 1.00 20.38	B	C
	ATOM	3489	CB		B 322	9.645	41.760	48.459 49.008	1.00 20.56	В	č
	ATOM	3490	CG		B 322	8.924 9.485	40.530	50.385	1.00 21.26	В	č
	ATOM	3491 3492	CD1		B 322 B 322	7.427	40.822	49.085	1.00 17.17	В	С
25	MOTA MOTA	3493	CD2		B 322	9.796	43.516	46.719	1.00 22.34	В	C
23	ATOM	3494	ŏ		B 322	9.027	44.451	46.927	1.00 23.00	В	0
	ATOM	3495	N	VAL	B 323	11.024	43.679	46.247	1.00 22.63	В	N
	ATOM	3496	CA		B 323	11.571	45.006	45.994	1.00 24.72	B	C
	ATOM	3497	CB		B 323	13.034	45.072 46.414	46.495 46.172	1.00 22.95 1.00 24.04	В	č
30	MOTA	3498	CG1		B 323	13.655	44.856	48.002	1.00 23.23	В	č
	ATOM	3499 3500	CG2 C		B 323 B 323	13.054 11.486	45.443	44.535	1.00 25.81	В	Ċ
	ATOM ATOM	3500	0		B 323	11.200	46.606	44.245	1.00 26.53	В	0
	ATOM	3502	N		в 324	11.730	44.516	43.617	1.00 25.39	В	N
35	ATOM	3503	CA		B 324	11.651	44.857	42.213	1.00 25.94	B	C
	ATOM	3504	С		B 324	12.980	44.762	41.508	1.00 26.51	В	C
	ATOM	3505	0		B 324	13.024	44.751	40.282	1.00 27.88	B B	N
	MOTA	3506	N	LYS	B 325 B 325	14.062 15.407	44.709	41.732	1.00 28.30	В	č
40	ATOM	3507 3508	CA	LYS	B 325	16.040	45.985	41.573	1.00 32.53	В	С
40	ATOM ATOM	3509	CG	LYS	B 325	16.057	46.809	42.843	1.00 36.71	В	С
	ATOM	3510	CD	LYS	B 325	16.678	48.183	42.605	1.00 41.59	В	c
	ATOM	3511	CE		B 325	16.621	49.053	43.864	1.00 44.11	B	C
	ATOM	3512	NZ		B 325	17.286	48.415	45.044 42.666	1.00 44.74 1.00 28.12	В	C
45	ATOM	3513	C		B 325 B 325	16.259 15.940	43.749	43.845	1.00 26.12	В	ŏ
	ATOM	3514 3515	N	PRO		17.348	43.160	42.147	1.00 26.86	В	N
	ATOM	3515	CD	PRO		17.790	43.134	40.742	1.00 26.79	В	С
	ATOM	3517	CA	PRO		18.212	42.330	42.991	1.00 26.22	В	C
50		3518	CB	PRO		19.137	41.653	41.979	1.00 27.30	B B	C
	ATOM	3519	CG	PRO		19.215	42.656 43.159	40.863 44.048	1.00 26.62 1.00 25.76	В	č
	MOTA	3520	C	PRO		18.952 19.249	44.330	43.838	1.00 24.87	В	ō
	ATOM	3521 3522	N	PRO		19.257	42.546		1.00 25.19	В	N
55		3522	CD	PRO		19.005	41.111	45.435	1.00 24.23	В	c
	ATOM	3524	CA	PRO		19.945	43.148	46.350	1.00 24.63	В	c
	ATOM	3525	CB	PRO		19.864	42.046		1.00 23.95	B B	C
	MOTA	3526	CG	PRO		19.947	40.801		1.00 24.61 1.00 25.54	В	c
	ATOM	3527	C	PRO		21.376	43.684		1.00 23.51	В	ŏ
60		3528 3529	N	PRO		21.766 22.158	43.128		1.00 27.17	В	N
	ATOM	3529	CA	PHE		23.540	43.572		1.00 27.57	В	С
	ATOM	3531	CB	PHE		24.480	42.365	45.205	1.00 24.24	В	c
	ATOM	3532	CG	PHE		24.257	41.519		1.00 23.37	В	c
65		3533	CD				41.964	47.694	1.00 21.17	B	C
	ATOM	3534	CD						1.00 20.04 1.00 19.30	В	c
	ATOM	3535							1.00 21.16	В	č
	ATOM	3536	CE	2 PHE					1.00 21.41	В	C
70	MOTA (3537 3538		PHE				43.786	1.00 30.91	В	C
/(ATOM	3539		PHE				43.424	1.00 29.74	В	0
	ATOM	3540			J B 329			43.073	1.00 35.49	В	N

3595

3597 С

3600 CA

3603

3605 ō

3606 N TYR B 337

3607

3610

OE1 GLU B 335

OE2 GLU B 335

OG1 THR B 336

CG2 THR B 336

CA TYR B 337

CG TYR B 337

CD1 TYR B 337

3611 CE1 TYR B 337 3612 CD2 TYR B 337

3601 CB THR B 336

GLU B 335

GLU B 335

THR B 336 THR B 336

THR B 336

55 ATOM

60 ATOM

65 ATOM

ATOM 3596

MOTA

ATOM 3598 0

MOTA 3599 N

MOTA

MOTA 3602

ATOM

MOTA 3604 С THR B 336

ATOM

ATOM

ATOM 3608 CB TYR B 337

ATOM 3609

MOTA

ATOM

70 ATOM

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	ATOM	3541	CA	GLU	В	320	22.809		41.792	1 00	39.40		В	C
	ATOM	3542	CB	GLU			21.422		41.257		40.82		В	C
	ATOM	3543	CG	GLU			21.439		39.829		44.77		В	c
	ATOM	3544	CD	GLU		329	20.104		39.401		45.81		В	c
5	ATOM	3545		GLU		329	19.695		39.986		46.10		В	Ö
-	ATOM	3546		GLU			19.465		38.480		47.31		В	0
	ATOM	3547	C	GLU			23.643		41.920		41.08		В	c
	ATOM	3548	ŏ	GLU			23.353		42.740		40.70		В	Ö
	ATOM	3549	N	ALA			24.686		41.106		43.84		B B	N
10	ATOM	3550	CA	ALA			25.554		41.120		46.89		В	C
10	MOTA	3551	CB	ALA			26.943	47.469	41.610		45.55		В	c
	ATOM	3552	c	ALA			25.633	48.417	39.709		49.66		В	c
	MOTA	3553	ŏ	ALA			25.028		38.776		50.00		В	Ö
	ATOM	3554	N	ASN			26.382		39.556		52.10			N
15	ATOM	3555	CA	ASN			26.531		38.256		54.10		B B	C
10	ATOM	3556	CB	ASN			26.785	51.634	38.436		55.63		В	c
	ATOM	3557	CG	ASN			26.419		37.205		57.22		В	č
	ATOM	3558		ASN			26.304		37.271		57.48		В	0
	ATOM	3559		ASN			26.240		36.074		58.16		В	N
20	ATOM	3560	C	ASN			27.691		37.513		54.40		В	C
	ATOM	3561	ŏ	ASN			27.748		36.286		54.29		В	Ö
	ATOM	3562	N	THR			28.602		38.266		55.19		3	N
	ATOM	3563	CA	THR			29.761		37.676		55.71		3	C
	ATOM	3564	CB	THR			31.056		37.908		55.73		В	č
25		3565		THR			32.189		37.491		56.87		В	Ö
	ATOM	3566		THR			31.210	49.385	39.371		55.37		В	č
	ATOM	3567	c	THR			29.977	46.787	38.206		56.55		В	č
	ATOM	3568	ŏ	THR			29.604		39.337		57.13		В	ŏ
	ATOM	3569	N	TYR			30.587		37.377		56.97		š	N
30	ATOM	3570	CA	TYR			30.861	44.558	37.739		56.81		3	ĉ
	ATOM	3571	CB	TYR			31.623	43.848	36.610		58.85		3	č
	ATOM	3572	CG	TYR			30.984	43.930	35.233		62.30		3	č
	MOTA	3573	CD1	TYR	В	333	31.675	43.490	34.099		62.80		3	č
	MOTA	3574	CE1	TYR	В	333	31.103	43.563	32.826		63.19		3	č
35	MOTA	3575	CD2	TYR	В	333	29.695	44.446	35.057	1.00	63.26		3	Ċ
	MOTA	3576	CE2	TYR	В	333	29.114	44.521	33.786	1.00	63.66	1	3	C
	MOTA	3577	CZ	TYR	В	333	29.825	44.079	32.678	1.00	63.50		3	С
	MOTA	3578	OH	TYR			29.257	44.153	31.425	1.00	63.78		3	0
	ATOM	3579	C	TYR			31.697	44.484	39.012	1.00	55.92	1	3	С
40	MOTA	3580	0	TYR			31.351	43.770	39.950	1.00	56.04		3	0
	MOTA	3581	N	GLN			32.802	45.224	39.033		55.18	1	3	N
	ATOM	3582	CA	GLN			33.711	45.227	40.176	1.00	54.38	1	3	С
	MOTA	3583	CB	GLN			34.871	46.203	39.925		55.19		3	C
	MOTA	3584	CG	GLN			34.482	47.678	39.879		57.42	1	3	C
45	MOTA	3585	CD	GLN			35.599	48.566	39.340		59.56	1	3	C
	MOTA	3586		GLN			36.756	48.459	39.759		60.33	1		0
	ATOM	3587		GLN			35.253	49.454	38.409		59.33	1		N
	ATOM	3588	С	GLN			32.998	45.572	41.478		53.11	1		C
	ATOM	3589	0	GLN			33.352	45.067	42.544		52.68	1		0
50	ATOM	3590	N	GLU			31.986	46.427	41.386		51.38	1		N
	ATOM	3591	CA	GLU			31.226	46.826	42.561		50.81	1		C
	ATOM	3592	CB	GLU			30.428	48.098	42.257		51.54		3	C
	ATOM	3593	CG	GLU			29.750	48.707	43.470		54.47	1		C
	ATOM	3594	CD	GLU			30.722	48.982	44.607	1.00	56.00	1	3	C

31.939 48.745

29.543 45.144

28.002 43.497

27.046 42.345

29.394 42.922

28.916 42.313

30.594 42.665

31.465 41.625 32.784 41.606

33.675 40.446

33.639 39.258

34.421 38.166

45.321 44.171

30.265 49.435

30.287 45.693

30.247

27.289 44.548

28.622 44.046

44.429

42.997

41.013

43.963

42.494

42.251

42.624

34.421 38.166 42.273 1.00 51.33 34.520 40.520 43.733 1.00 49.23

1.00 56.77

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1.00 48.26

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1.00 45.11 1.00 47.49

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45.681 1.00 55.50

42.042 1.00 47.63 42.318 1.00 46.12

40.347 1.00 47.48 41.308 1.00 44.35

43.001 1.00 45.04

43.025 1.00 42.44

41.901 1.00 48.63

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	ATOM	3613	CE2	TYR	B 337	35.302	39.439	44.114	1.00 50.54	В	C
	ATOM	3614	CZ		B 337	35.247	38.263	43.380	1.00 51.96	В	C
	ATOM	3615	OH		B 337	36.005	37.179	43.761	1.00 54.44	В	0
5	ATOM	3616	C		В 337	31.769	41.809	44.513	1.00 41.13	В	C
5	ATOM ATOM	3617 3618	0		B 337 B 338	31.759 32.048	40.843	45.276	1.00 40.24	B	0
	ATOM	3618	N CA		B 338	32.048	43.050 43.390	44.909 46.296	1.00 40.20 1.00 38.23	В	C N
	ATOM	3620	CB	LYS		32.833	44.850	46.388	1.00 41.59	В	č
	ATOM	3621	CG	LYS		34.123	45.176	45.644	1.00 44.66	В	č
10	ATOM	3622	CD		B 338	34.527	46.631	45.891	1.00 48.09	В	č
	ATOM	3623	CE		B 338	35.874	46.981	45.256	1.00 48.00	В	C
	ATOM	3624	NZ		B 338	35.838	46.925	43.765	1.00 51.10	В	N
	ATOM	3625	C		B 338	31.205	43.191	47.262	1.00 35.20	В	C
15	ATOM	3626 3627	и		B 338 B 339	31.339 30.063	42.526 43.783	48.291 46.923	1.00 32.57 1.00 33.78	B B	O N
	ATOM	3628	CA		B 339	28.868	43.694	47.758	1.00 32.18	В	C
	MOTA	3629	CB		B 339	27.741	44.499	47.125	1.00 34.50	В	č
	ATOM	3630	CG	ARG	B 339	28.069	45.975	46.971	1.00 34.49	В	C
	MOTA	3631	CD		B 339	26.849	46.753	46.513	1.00 37.43	В	C
20	MOTA	3632	NE		B 339	27.183	48.140	46.215	1.00 39.07	В	N
	MOTA	3633 3634	CZ		B 339 B 339	26.318	49.042	45.768	1.00 40.69	B	C
	ATOM	3635			B 339	25.052 26.723	48.714 50.278	45.563 45.524	1.00 41.15 1.00 42.78	В	N
	ATOM	3636	C		B 339	28.424	42.255	48.005	1.00 30.59	В	C
25	ATOM	3637	ō	ARG		27.998	41.916	49.106	1.00 30.06	В	ō
	ATOM	3638	N	ILE		28.531	41.411	46.983	1.00 28.84	В	N
	ATOM	3639	CA		B 340	28.172	40.005	47.113	1.00 28.23	В	C
	MOTA	3640	CB		B 340	28.265	39.284	45.746	1.00 29.04	В	C
30	ATOM ATOM	3641 3642	CG2 CG1	ILE	B 340 B 340	28.191 27.143	37.777	45.932 44.828	1.00 27.61 1.00 29.93	В	C
30	ATOM	3643	CD1		B 340	27.143	39.778	44.828	1.00 29.93	B B	c
	ATOM	3644	C		B 340	29.149	39.362	48.094	1.00 28.00	В	č
	ATOM	3645	o		B 340	28.746	38.760	49.092	1.00 28.08	В	ō
	ATOM	3646	N	SER		30.437	39.511	47.806	1.00 27.83	В	N
35	ATOM	3647	CA	SER		31.500	38.971	48.647	1.00 27.74	В	C
	ATOM	3648	CB	SER		32.869	39.405	48.099	1.00 29.39	В	c
	ATOM	3649 3650	OG C	SER		33.904 31.390	39.101	49.023 50.115	1.00 31.17 1.00 26.62	B B	0
	ATOM	3651	ö	SER		31.581	38.576	51.019	1.00 26.60	В	ŏ
40	ATOM	3652	N		B 342	31.095	40.670	50.349	1.00 26.86	В	N
	ATOM	3653	CA		B 342	30.967	41.190	51.713	1.00 27.32	В	C
	ATOM	3654	CB		B 342	31.486	42.635	51.786	1.00 30.87	В	C
	ATOM	3655	CD		B 342	32.988	42.792	51.559	1.00 34.75	B	C
45	ATOM	3656 3657	NE	ARG	B 342 B 342	33.407 34.861	44.264 44.410	51.585 51.496	1.00 38.59 1.00 44.23	В	N
73	ATOM	3658	CZ		B 342	35.518	45.568	51.542	1.00 45.71	В	Č
	ATOM	3659	NH1		B 342	36.842	45.574	51.450	1.00 47.72	В	N
	ATOM	3660	NH2		B 342	34.862	46.717	51.678	1.00 45.74	В	N
	ATOM	3661	С	ARG		29.525	41.157	52.232	1.00 26.65	В	C
50	ATOM	3662	O N	ARG VAL		29.249	41.651	53.324	1.00 24.28	В	0
	ATOM ATOM	3663 3664	CA	VAL		28.615 27.201	40.578 40.491	51.449 51.825	1.00 25.25 1.00 23.45	В	N
	ATOM	3665	CB	VAL		26.964	39.453	52.942	1.00 22.70	В	č
	ATOM	3666	CG1	VAL		25.475	39.151	53.038	1.00 26.95	В	č
55	ATOM	3667	CG2	VAL		27.744	38.182	52.667	1.00 24.45	В	C
	ATOM	3668	C	VAL		26.667	41.834	52.319	1.00 22.20	В	C
	ATOM	3669	0	VAL		26.236	41.958	53.463	1.00 22.42	В	0
	ATOM ATOM	3670 3671	N CA	GLU		26.702 26.224	42.841 44.163	51.461 51.836	1.00 20.93 1.00 19.95	B B	N
60	ATOM	3672	CB	GLU		27.317	45.217	51.593	1.00 21.95	В	c
	ATOM	3673	CG	GLU		28.483	45.077	52.579	1.00 26.85	В	c
	ATOM	3674	CD	\mathbf{GLU}	B 344	29.731	45.844	52.177	1.00 29.55	В	C
	MOTA	3675	OE1	GLU		30.643	45.948	53.029	1.00 31.16	В	0
	ATOM	3676	OE2	GLU		29.811	46.331	51.021	1.00 29.15	В	0
65	ATOM ATOM	3677 3678	C	GLU		24.970 25.007	44.500 44.692	51.054 49.832	1.00 19.08 1.00 15.34	B	C
	ATOM	3679	O N		B 344 B 345	23.859	44.555	51.778	1.00 16.62	В	N
	ATOM	3680	CA		B 345	22.572	44.858	51.778	1.00 19.25	В	C
	ATOM	3681	CB	PHE	B 345	21.938	43.576	50.615	1.00 17.18	В	C
70	MOTA	3682	CG		B 345	21.524	42.574	51.661	1.00 17.47	В	C
	MOTA	3683		PHE		20.271	42.645	52.253	1.00 18.52	В	C
	MOTA	3684	CD2	PHE	B 345	22.394	41.561	52.060	1.00 19.11	В	C

							-96-				
	ATOM	3685	CE1	PHE E	3 4 5	19.884	41.725	53.225	1.00 18.14	В	c
	ATOM	3686	CE2	PHE E	345	22.015	40.634	53.039	1.00 20.48	В	č
	ATOM	3687	$^{\rm cz}$	PHE E		20.758	40.719	53.620	1.00 19.36	В	C
	ATOM	3688	C	PHE E		21.673	45.470	52.253	1.00 18.97	В	C
5	ATOM	3689 3690	N	THR E		21.857	45.229	53.450	1.00 19.32	B	0
	ATOM	3691	CA	THR E		20.714 19.775	46.275 46.917	51.811 52.715	1.00 19.42 1.00 19.27	В	N
	ATOM	3692	CB	THR E		20.082	48.424	52.715	1.00 19.27	В	c
	ATOM	3693	OG1	THR E		20.109	49.030	51.564	1.00 20.30	В	ō
10	ATOM	3694	CG2	THR E		21.437	48.635	53.539	1.00 18.82	В	c
	ATOM	3695	C	THR E		18.350	46.704	52.197	1.00 19.39	В	C
	ATOM	3696	0	THR E		18.163	46.200	51.095	1.00 20.35	B	0
	ATOM	3697	N CA	PHE E		17.364	47.086	53.003	1.00 20.32	В	N
15	ATOM	3698 3699	CB	PHE E		15.941 15.239	46.925 46.134	52.689 53.801	1.00 22.26	В	C
13	ATOM	3700	CG	PHE E		15.710	44.715	53.954	1.00 19.26 1.00 22.00	B B	C
	ATOM	3701		PHE E		15.318	43.731	53.050	1.00 20.34	В	č
	ATOM	3702		PHE E		16.521	44.352	55.029	1.00 19.14	В	č
	ATOM	3703		PHE E		15.723	42.411	53.217	1.00 18.46	В	C
20	MOTA	3704	CE2	PHE E		16.930	43.037	55.202	1.00 16.81	В	С
	ATOM	3705	CZ	PHE E		16.529	42.062	54.293	1.00 16.52	В	C
	ATOM ATOM	3706 3707	C	PHE E		15.180 15.384	48.246	52.572	1.00 23.77	В	C
	ATOM	3708	N	PRO B		14.280	49.166 48.353	53.364 51.590	1.00 24.75 1.00 26.17	B B	N O
25	ATOM	3709	CD	PRO E		14.032	47.471	50.438	1.00 27.03	В	C
	ATOM	3710	CA	PRO E		13.519	49.602	51.474	1.00 27.72	В	č
	ATOM	3711	CB	PRO B	348	12.702	49.393	50.198	1.00 28.07	В	C
	ATOM	3712	CG	PRO B		13.561	48.455	49.394	1.00 28.17	В	C
20	ATOM	3713	C	PRO B		12.629	49.609	52.727	1.00 29.25	В	C
30	ATOM	3714	O N	PRO B		12.262	48.546	53.232	1.00 29.40	В	0
	ATOM	3715 3716	CA	ASP B		12.265 11.453	50.784 50.864	53.220 54.426	1.00 30.11	B B	N C
	ATOM	3717	CB	ASP B		11.199	52.329	54.785	1.00 35.47	В	c
	ATOM	3718	CG	ASP B	349	12.486	53.141	54.863	1.00 39.29	В	č
35	ATOM	3719	OD1	ASP B		13.519	52.592	55.315	1.00 40.71	В	ō
	ATOM	3720		ASP B		12.463	54.334	54.483	1.00 42.81	В	0
	ATOM	3721	C	ASP B		10.127	50.105	54.428	1.00 30.99	В	C
	ATOM	3722 3723	N O	ASP B		9.639	49.729	55.501	1.00 31.13	В	õ
40	ATOM	3724	CA	PHE B		9.539 8.256	49.858 49.153	53.256 53.225	1.00 28.24	B	N
	ATOM	3725	CB	PHE B		7.496	49.459	51.920	1.00 21.72	В	č
	ATOM	3726	CG	PHE B	350	8.175	48.964	50.670	1.00 20.48	В	č
	ATOM	3727		PHE B		8.133	47.616	50.323	1.00 20.47	В	C
45	ATOM	3728		PHE B		8.836	49.853	49.825	1.00 18.76	В	C
43	ATOM	3729 3730	CE1	PHE B		8.741 9.447	47.156 49.412	49.145 48.649	1.00 19.61	B B	C
	ATOM	3731	CZ	PHE B		9.447	49.412	48.849	1.00 20.75	В	c
	ATOM	3732	c	PHE B		8.327	47.637	53.442	1.00 25.64	В	č
	ATOM	3733	0	PHE B	350	7.293	47.002	53.660	1.00 25.56	В	ō
50	ATOM	3734	N	VAL B		9.523	47.050	53.386	1.00 23.17	В	N
	ATOM	3735	CA	VAL B		9.643	45.604	53.586	1.00 21.29	В	С
	ATOM	3736 3737	CB CG1	VAL B		11.012 11.060	45.072 43.564	53.124 53.314	1.00 18.96 1.00 18.55	B B	C
	ATOM	3738	CG2	VAL B		11.244	45.423	51.663	1.00 15.50	В	c
55	ATOM	3739	C	VAL B		9.429	45.215	55.052	1.00 21.74	В	č
	ATOM	3740	0	VAL B	351	10.054	45.772	55.949	1.00 20.28	В	ō
	MOTA	3741	N	THR B		8.535	44.254	55.273	1.00 22.77	В	N
	MOTA	3742	CA	THR B		8.186	43.776	56.609	1.00 23.82	В	C
60	ATOM	3743 3744	CB OG1	THR B		6.918 5.829	42.899	56.523 56.054	1.00 25.23	В	C
00	ATOM	3744		THR B		6.555	42.331	57.872	1.00 27.41 1.00 27.51	B	0
	ATOM	3746	C	THR B		9.304	43.017	57.343	1.00 27.51	В	c
	ATOM	3747	ŏ	THR B		10.213	42.463	56.718	1.00 23.44	В	Ö
	ATOM	3748	N	ALA B		9.228	42.998	58.674	1.00 22.56	В	N
65	MOTA	3749	CA	ALA B		10.233	42.334	59.502	1.00 19.72	В	C
	ATOM	3750	CB	ALA B		10.018	42.682	60.984	1.00 21.49	В	C
	ATOM ATOM	3751 3752	C	ALA B		10.230 11.270	40.825	59.305 59.390	1.00 18.37 1.00 17.81	B	C
	ATOM	3753	N	GLY B	354	9.061	40.184	59.390	1.00 17.81	В	N O
70	ATOM	3754	CA	GLY B		9.002	38.820	58.807	1.00 14.69	В	C
	ATOM	3755	C	GLY B		9.749	38.486	57.524	1.00 15.67	В	č
	ATOM	3756	0	GLY B		10.484	37.497	57.449	1.00 15.82	В	ŏ

							-97-				
	MOTA	3757	N	ALA	B 355	9.571	39.318	56.503	1.00 14.39	В	N
	ATOM	3758	CA	ALA		10.241	39.091	55.227	1.00 16.28	В	C
	ATOM	3759 3760	CB C	ALA		9.683	40.047	54.163	1.00 14.46	В	C
5	ATOM	3761	0	ALA		11.759 12.541	39.285 38.560	55.374 54.778	1.00 16.62 1.00 18.69	B	C
	ATOM	3762	N		B 356	12.162	40.266	56.175	1.00 18.54	В	N
	ATOM	3763	CA		B 356	13.571	40.558	56.397	1.00 18.70	В	c
	ATOM	3764	CB		B 356	13.703	41.894	57.138	1.00 19.52	В	C
10	ATOM	3765	CG		B 356	13.122	43.053	56.343	1.00 21.00	В	С
10	MOTA	3766 3767	CD	ARG	B 356 B 356	12.584 13.576	44.189 45.223	57.208	1.00 21.75	В	С
	ATOM	3768	CZ	ARG		13.435	46.503	57.463 57.130	1.00 25.09 1.00 20.74	B	N C
	ATOM	3769	NH1			12.340	46.921	56.528	1.00 23.41	В	N
	ATOM	3770	NH2	ARG		14.400	47.363	57.394	1.00 19.75	В	N
15	MOTA	3771	C	ARG		14.266	39.436	57.168	1.00 20.44	B	C
	MOTA	3772	0	ARG		15.449	39.156	56.951	1.00 21.10	В	0
	ATOM ATOM	3773 3774	N CA		B 357 B 357	13.546	38.786	58.076	1.00 20.86	В	N
	ATOM	3775	CB		B 357	14.164 13.259	37.698 37.204	58.819 59.938	1.00 18.80 1.00 20.18	B B	C
20	MOTA	3776	CG		B 357	13.911	36.098	60.740	1.00 19.17	В	č
	ATOM	3777	OD1		B 357	14.805	36.415	61.543	1.00 20.57	В	ō
	ATOM	3778	OD2		B 357	13.552	34.918	60.555	1.00 21.02	В	0
	MOTA	3779	c		B 357	14.465	36.530	57.887	1.00 18.01	В	C
25	MOTA	3780 3781	O		B 357 B 358	15.539 13.508	35.937 36.199	57.941 57.029	1.00 19.94 1.00 18.45	B	O N
23	ATOM	3782	CA	LEU		13.696	35.101	56.087	1.00 17.99	В	C
	ATOM	3783	CB		B 358	12.442	34.900	55.231	1.00 17.24	В	č
	MOTA	3784	CG	LEU	B 358	12.619	33.829	54.153	1.00 18.71	В	С
30	MOTA	3785			B 358	12.858	32.466	54.819	1.00 17.61	В	C
30	ATOM ATOM	3786 3787		LEU		11.396	33.791	53.254	1.00 20.87	В	C
	ATOM	3788	c	LEU	B 358 B 358	14.879 15.745	35.357 34.499	55.161 54.986	1.00 17.62 1.00 17.62	B	C
	ATOM	3789	N		B 359	14.906	36.543	54.565	1.00 16.22	В	N
	ATOM	3790	CA	ILE	B 359	15.976	36.891	53.640	1.00 19.15	В	С
35	ATOM	3791	CB		B 359	15.684	38.236	52.940	1.00 18.39	В	C
	ATOM	3792			B 359	16.848	38.610	52.036	1.00 17.22	В	C
	ATOM	3793 3794	CG1		B 359 B 359	14.387 13.872	38.117 39.439	52.129 51.528	1.00 20.22 1.00 22.11	B	C
	ATOM	3795	CDI		B 359	17.363	36.947	54.282	1.00 22.11	В	č
40	ATOM	3796	ō		B 359	18.359	36.611	53.640	1.00 16.11	В	ŏ
	ATOM	3797	N		B 360	17.433	37.364	55.543	1.00 16.97	В	N
	ATOM	3798	CA		B 360	18.725	37.447	56.213	1.00 18.07	В	С
	ATOM ATOM	3799 3800	CB OG	SER	B 360 B 360	18.615 18.402	38.316 39.669	57.466 57.111	1.00 18.16 1.00 17.16	B	C
45	MOTA	3801	C	SER		19.267	36.060	56.573	1.00 17.18	В	č
	ATOM	3802	ō		B 360	20.480	35.874	56.711	1.00 18.93	В	ŏ
	ATOM	3803	N		B 361	18.369	35.088	56.716	1.00 19.00	В	N
	ATOM	3804	CA	ARG		18.775	33.730	57.040	1.00 20.67	В	С
50	ATOM ATOM	3805 3806	CB	ARG		17.630 17.160	33.003	57.742 58.993	1.00 25.65 1.00 31.87	В	C
50	ATOM	3807	CD		B 361	16.083	32.947	59.716	1.00 31.87	B B	C
	ATOM	3808	NE	ARG		16.529	31.589	59.998	1.00 44.86	В	N
	MOTA	3809	CZ		B 361	15.896	30.743	60.804	1.00 48.17	В	C
	ATOM	3810			B 361	14.779	31.116	61.419	1.00 47.35	В	N
55	ATOM ATOM	3811 3812	NH2 C		B 361 B 361	16.382	29.521	60.993	1.00 48.87	В	N
	ATOM	3813	Ö		B 361	19.211 19.994	32.974	55.785 55.855	1.00 21.43 1.00 22.60	B	C
	MOTA	3814	N		B 362	18.721	33.407	54.628	1.00 20.42	В	N
	ATOM	3815	CA	LEU	B 362	19.087	32.763	53.375	1.00 18.53	В	c
60	MOTA	3816	CB		B 362	17.949	32.888	52.362	1.00 17.29	В	C
	ATOM	3817	CG		B 362	16.665	32.103	52.653	1.00 15.10	В	C
	MOTA	3818 3819	CD1		B 362 B 362	15.621 16.961	32.437	51.611 52.650	1.00 15.28 1.00 14.06	В	C
	ATOM	3820	CDZ		B 362	20.364	33.370	52.650	1.00 14.06	B	C
65	ATOM	3821	ŏ		B 362	21.117	32.695	52.090	1.00 19.39	В	ō
	MOTA	3822	N		B 363	20.614	34.640	53.098	1.00 19.15	В	N
	MOTA	3823	CA		B 363	21.793	35.310	52.565	1.00 21.61	В	C
	ATOM ATOM	3824 3825	CB		B 363 B 363	21.421 20.391	36.728 36.784	52.121 50.986	1.00 21.25 1.00 22.02	В	C
70	ATOM	3826		LEU		20.391	38.228	50.986	1.00 22.02	B B	C
	MOTA	3827		LEU		20.941	36.079	49.732	1.00 21.42	В	c

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	MOTA	3829	0	LEU			23.4		36.421 34.158	53.931		25.25	B B	0
	ATOM	3830 3831	N CA	LYS			23.4 24.5		34.004	53.939 54.860		22.72	В	N C
	ATOM	3832	CB	LYS			24.2		32.822	55.812		26.10	B	c
5	ATOM	3833	CG	LYS			23.3		33.116	56-964	1.00	28.20	В	č
	ATOM	3834	CD	LYS	В	364	23.9	70	34.044	57.987	1.00	30.83	В	C
	ATOM	3835	CE	FAR		364	22.9		34.630	58.974		33.43	В	C
	MOTA	3836	NZ	LYS		364	22.3		33.622	59.900	1.00	36.33	В	N
10	ATOM	3837 3838	C	LYS		364 364	25.8 25.8		33.766 32.987	54.062 53.102		25.33	B	C
10	ATOM	3839	N	HIS		365	26.9	n4	34.444	54.455		25.93	B	N
	ATOM	3840	CA	HIS		365	28.1	75	34.296	53.763		26.63	В	c
	ATOM	3841	CB	HIS		365	29.2		35.141	54.424		25.92	В	C
	ATOM	3842	CG	HIS		365	30.5		35.009	53.756		26.63	В	C
15	MOTA	3843		HIS			31.6		34.202	54.022		25.39	В	C
	MOTA	3844		HIS			30.9		35.688	52.598		28.19	В	N
	MOTA	3845 3846			B B	365 365	32.1 32.5	03	35.303	52.179 53.024		27.11 26.10	B B	N C
	ATOM	3847	C	HIS		365	28.6	36	32.845	53.757		26.18	В	Ç
20	ATOM	3848	ŏ		В	365	29.1		32.338	52.747		27.21	В	ŏ
	ATOM	3849	N	ASN		366	28.5		32.195	54.907	1.00	27.62	В	N
	ATOM	3850	CA	ASN		366	28.9		30.804	55.076	1.00	29.77	В	C
	ATOM	3851	CB		В	366	29.4		30.620	56.493	1.00	31.38	В	C
25	ATOM	3852	CG		В	366	29.7		29.190	56.802	1.00	35.31	В	C
23	ATOM ATOM	3853 3854			B B	366 366	30.3 29.4		28.480 28.757	55.963 58.020	1.00	38.20 37.60	B B	N
	ATOM	3855	C		В	366	27.7		29.862	54.805	1.00	28.07	В	C
	ATOM	3856	ŏ		B	366	26.7		29.793	55.583	1.00	26.33	B	ŏ
	ATOM	3857	N		в	367	27.7		29.121	53.690	1.00	29.03	В	N
30	ATOM	3858	CD		В	367	28.9		29.001	52.804	1.00	29.75	В	C
	ATOM	3859	CA		В	367	26.7		28.182	53.285	1.00	29.22	В	C
	ATOM	3860	CB		В	367	27.2		27.542	52.017	1.00	27.84	В	C
	ATOM	3861 3862	CG		B	367 367	28.7 26.2		27.619 27.148	52.224 54.323	1.00	29.93	B B	c
35	ATOM	3863	ŏ		B	367	25.1		26.715	54.332		30.60	В	o
	ATOM	3864	N	SER		368	27.2		26.754	55.198	1.00	30.30	B	N
	ATOM	3865	CA		В	368	26.8	71	25.762	56.208	1.00	31.18	В	C
	ATOM	3866	CB	SER		368	28.1	41	25.252	56.905	1.00	32.85	В	C
40	ATOM	3867	C	SER		368	28.5 25.9		26.132 26.345	57.939	1.00	35.93	B	0
40	ATOM	3868 3869	0	SER	B	368 368	25.2		25.613	57.233 57.975	1.00	30.36	В	C
	ATOM	3870	N		В	369	25.7		27.667	57.264		31.55	В	N
	ATOM	3871	CA	GLN		369	24.8		28.333	58.200	1.00	32.07	В	c
	ATOM	3872	CB		В	369	25.5		29.665	58.656		36.11	В	C
45	ATOM	3873	CG		В	369	26.8		29.518	59.359		42.42	В	C
	ATOM	3874 3875	CD		В	369 369	27.3 26.7		30.837	59.891 60.766	1.00	45.10 48.57	B	C
	ATOM	3876		GLN	B	369	28.5		31.454	59.361	1.00	46.32	В	N
	ATOM .	3877	C	GLN		369	23.5		28.581	57.618		29.24	В	C
50	ATOM	3878	ō	GLN		369	22.6		29.029	58.323		28.91	В	ō
	ATOM	3879	N	ARG		370	23.3		28.301	56.331		27.41	В	N
	ATOM	3880	CA		В	370	22.0	36	28.496	55.675		25.29	В	C
	ATOM	3881	CB		В	370	22.2		28.548	54.157 53.698		23.14	B B	C
55	ATOM	3882 3883	CD	ARG		370 370	23.5		29.715	52.268		21.09	B	č
55	ATOM	3884	NE	ARG		370	24.6		30.468	51.956		20.83	В	N
	ATOM	3885	CZ		B	370	25.4		30.365	50.895		22.00	В	c
	ATOM	3886			В	370	25.2	35	29.372	50.029		21.78	В	N
	ATOM	3887		ARG	В	370	26.3		31.262	50.698		23.58	В	N
60		3888	C	ARG		370	21.0	96	27.348	56.048		24.43	В	C
	ATOM	3889 3890	O N	ARG PRO		370 371	21.5 19.7	33	26.214 27.625	56.209 56.177		25.53 25.63	В	O N
	ATOM	3890	CD		В	371	19.7		28.920	55.965		25.62	B	C
	ATOM	3892	CA		В	371	18.8		26.584	56.538		25.56	В	č
65	ATOM	3893	CB	PRO	в	371	17.5	61	27.392	56.860	1.00	25.65	В	C
	MOTA	3894	CG		в	371	17.6	49	28.519	55.882	1.00	24.95	В	C
	ATOM	3895	C		В	371	18.5	51	25.529	55.461		25.92	В	C
	ATOM	3896	O	PRO	В	371 372	18.9		25.689	54.308		27.40	В	0
70	ATOM	3897 3898	N CA	MET	В	372	17.8 17.5		24.444	55.853 54.911	1.00	27.14	В	N
, 0	ATOM	3899	CB		В	372	17.3		22.053	55.623		29.21	В	c
	ATOM	3900	CG	MET			18.6		21.462	56.225		32.29	В	c
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	MOTA	3901	SD	MET			18.257	19.888	57.038	1.00	38.80	1	3	s
	MOTA	3902	CE	MET			18.599	18.751	55.690		36.16	1		C
	MOTA	3903 3904	C	MET			16.206	23.820	54.305		26.36		3	C
5	MOTA	3904	O N	LEU			15.471 15.901	24.590 23.323	54.922 53.108		27.49		В В	N
-	ATOM	3906	CA	LEU			14.657	23.663	52.423		22.39		3	c
	MOTA	3907	CB	LEU			14.528	22,850	51.132		22.84		3	č
	MOTA	3908	CG	LEU	В	373	15.511	23.250	50.032	1.00	24.40	1	3	C
	MOTA	3909		LEU			15.332	22.333	48.825		26.89		3	С
10	ATOM	3910		PEA			15.282	24.716	49.638		24.98		3	C
	MOTA	3911 3912	C	LEU			13.412 12.488	23.470 24.280	53.272 53.212		20.58		3	C
	ATOM	3913	N	ALA			13.393	22.409	54.071		21.21		3	N
	ATOM	3914	CA	ALA	В	374	12.249	22.111	54.936		23,10		3	c
15	ATOM	3915	CB	ALA			12.423	20.733	55.580		26.30		3	C
	ATOM	3916	C	ALA			12.033	23.168	56.019		23.37		3	C
	MOTA	3917	0			374	10.916	23.353	56.496		23.95		3	0
	ATOM	3918 3919	N CA	GLU	В	375 375	13.102 13.007	23.854	56.410 57.426		22.62		3	И
20	ATOM	3920	CB	GLU			14.394	25.218	57.984		23.52		3	č
	ATOM	3921	CG		В		15.035	24.067	58.761		27.91		3	č
	ATOM	3922	CD	GLU			16.465	24.369	59.174		29.27		3	č
	MOTA	3923	OE1				16.666	25.158	60.120	1.00	31.60		3	0
0.5	MOTA	3924		GLU			17.389	23.826	58.538		29.51		3	0
25	MOTA MOTA	3925 3926	C	GLU			12.380 11.661	26.139 26.874	56.823 57.497		22.31		3	C
	ATOM	3927	N			376	12.664	26.376	55.545		21.78		3	N
	ATOM	3928	CA			376	12.106	27.526	54.840		21.13		3	č
	MOTA	3929	CB			376	12.666	27.613	53.394		18.71		3	С
30	MOTA	3930		VAL			11.973	28.725	52.634		17.37		3	С
	ATOM	3931		VAL		376	14.176	27.854	53.429		15.43		3	С
	ATOM ATOM	3932 3933	C	VAL		376 376	10.582 9.841	27.378 28.336	54.777 55.006		22.45		3	C
	ATOM	3934	N	LEU		377	10.133	26.163	54.478		22.30		3	N
35	ATOM	3935	CA	LEU		377	8.715	25.857	54.366		26.34		3	ċ
	ATOM	3936	CB	LEU	В	377	8.533	24.449	53.785		26.41	1	3	C
	MOTA	3937	CG	LEU		377	9.025	24.299	52.343		27.84	1		С
	MOTA	3938			В	377	9.044	22.837	51.924		27.54	1		C
40	MOTA	3939 3940	CD2	LEU		377 377	8.115 7.976	25.105 25.971	51.431 55.693		26.87 27.31	1		C
-10	ATOM	3941	ŏ	LEU		377	6.752	25.965	55.719		28.00		3.	õ
	ATOM	3942	N	GLU		378	8.722	26.069	56.788		27.51	i		N
	ATOM	3943	CA	$_{\rm GLU}$		378	8.126	26.189	58.113		28.70	1	3	С
	ATOM	3944	CB	GLU		378	8.796	25.221	59.100		33.15		3	C
45	ATOM	3945 3946	CD	GLU		378 378	8.265 9.030	23.796	59.082 60.036		39.47	1		C
	ATOM	3947	OE1	GLU			8.545	21.758	60.311		47.53			Ö
	ATOM	3948	OE2				10.119	23.271	60.506		44.23			ŏ
	ATOM	3949	C	GLU	В	378	8.252	27.601	58.659		26.28	1	3	Ċ
50	ATOM	3950	0	GLU		378	7.780	27.886	59.752		26.40	1		0
	ATOM	3951	N	HIS	В		8.891	28.491	57.915		23.55	1		N
	ATOM	3952 3953	CB	HIS			9.045 9.891	29.852 30.671	58.405 57.438		22.18 18.53	1		C
	ATOM	3954	CG	HIS			10.310	31.999	57.984		20.37			č
55	ATOM	3955		HIS			11.503	32.430	58.455	1.00	16.86	i		č
	ATOM	3956		HIS			9.437	33.058	58.121	1.00	18.83	1		N
	ATOM	3957		HIS			10.076	34.084	58.653		19.47	1		С
	ATOM	3958 3959	NE2	HIS			11.330	33.729	58.864		20.07	1		N
60	ATOM	3960	ŏ	HIS	B	379	7.672 6.784	30.488	58.604 57.760		22.39	1		C
	ATOM	3961	N	PRO			7.477	31.199	59.734		21.58	- 1		N
	ATOM	3962	CD	PRO	в	380	8.461	31.340	60.818		20.38	i	3	С
	ATOM	3963	CA	PRO			6.218	31.870	60.091		20.86	1		C
ce	ATOM	3964	CB	PRO			6.521	32.487	61.458		22.72	1		С
65	ATOM ATOM	3965 3966	CG	PRO			7.574	31.573	62.013		23.24	1		C
	ATOM	3966	0	PRO			5.697 4.483	32.910 33.127	59.095 59.013		21.33 17.95	1		C
	ATOM	3968	N	TRP			6.599	33.560	58.355		19.60	í		N
	ATOM	3969	CA	TRP	В	381	6.183	34.555	57.365	1.00	19.09	i		С
70	ATOM	3970	CB	TRP			7.373	35.392	56.893		19.18	1		C
	ATOM	3971	CG			381	7.000	36.467	55.892		20.21	1		C
	ATOM	3972	CD2	TRP	в	381	7.254	36.450	54.478	1.00	18.07	1	3	C

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	ATOM	3973	CE2	TRP	B 381	6.688	37.629	53.935	1.00 18.87	В	C
	ATOM	3974			B 381	7.901	35.554	53.619	1.00 19.02	В	C
	MOTA	3975			B 381	6.316	37.630	56.142	1.00 18.93	В	C
5	ATOM ATOM	3976 3977	CZ2		B 381 B 381	6.126 6.748	38.331 37.929	54.970 52.570	1.00 16.23 1.00 16.90	B	N
ر	ATOM	3978	CZ3		B 381	7.962	35.855	52.570	1.00 18.90	В	C
	ATOM	3979			B 381	7.386	37.034	51.747	1.00 17.42	В	č
	ATOM	3980	C		B 381	5.572	33.809	56.171	1.00 20.19	В	C
	ATOM	3981	0		B 381	4.562	34.233	55.600	1.00 16.91	В	0
10	ATOM	3982	N		B 382	6.199	32.699	55.801	1.00 18.76	В	N
	ATOM	3983 3984	CB		B 382 B 382	5.719 6.766	31.887 30.844	54.695 54.318	1.00 22.56	B B	c
	ATOM	3985			B 382	6.139	29.747	53.486	1.00 22.31	В	c
	ATOM	3986			B 382	7.908	31.529	53.573	1.00 23.31	В	č
15	ATOM	3987			B 382	9.066	30.636	53.321	1.00 29.66	В	Ċ
	ATOM	3988	C		B 382	4.395	31.181	55.019	1.00 24.58	В	C
	MOTA	3989	0		в 382	3.447	31.210	54.230	1.00 23.86	В	0
	ATOM ATOM	3990 3991	N CA		B 383 B 383	4.348	30.543	56.183 56.640	1.00 25.64	B B	N
20	ATOM	3991	CB		B 383	3.462	29.825 29.123	57.982	1.00 25.76	В	C
20	ATOM	3993		THR		4.162	27.896	57.732	1.00 31.20	В	Ö
	ATOM	3994		THR		2.196	28.841	58.734	1.00 28.47	В	č
	ATOM	3995	С		B 383	1.966	30.746	56.812	1.00 26.92	В	C
	ATOM	3996	0		в 383	0.817	30.336	56.615	1.00 27.54	В	0
25	ATOM	3997	N		B 384	2.234	31.994	57.175	1.00 26.10	В	N
	MOTA	3998 3999	CB		B 384 B 384	1.170 1.653	32.961 34.053	57.396 58.326	1.00 27.17 1.00 25.11	B B	C
	ATOM	4000	c		B 384	0.635	33.584	56.119	1.00 28.32	В	c
	ATOM	4001	ō		B 384	-0.550	33.900	56.022	1.00 27.86	В	ŏ
30	ATOM	4002	N		B 385	1.503	33.756	55.134	1.00 29,11	· B	N
	ATOM	4003	CA		в 385	1.090	34.392	53.898	1.00 32.57	В	C
	ATOM	4004	CB		в 385	2.128	35.451	53.541	1.00 27.65	В	C
	ATOM ATOM	4005 4006	CG		B 385 B 385	2.247 1.328	36.512 37.303	54.625 54.829	1.00 26.99	B B	C
35	ATOM	4007			B 385	3.367	36.517	55.342	1.00 23.20	В	N
	ATOM	4008	c		B 385	0.807	33.447	52.735	1.00 35.05	В	Ĉ
	ATOM	4009	0		B 385	0.812	33.859	51.580	1.00 35.34	В	0
	ATOM	4010	N		B 386	0.527	32.190	53.078	1.00 40.53	В	N
40	ATOM ATOM	4011 4012	CA		B 386 B 386	0.201	31.117	52.138	1.00 44.93	B B	C
40	ATOM	4012	OG		B 386	-0.537 -0.956	31.661	50.910 50.055	1.00 45.41	В	C
	ATOM	4014	C		B 386	1.436	30.343	51.701	1.00 48.13	В	č
	ATOM	4015	ŏ		в 386	2.357	30.904	51.108	1.00 48.75	В	ŏ
	ATOM	4016	N	SER :	B 387	1.435	29.046	52.006	1.00 51.11	В	N
45	ATOM	4017	CA		B 387	2.536	28.143	51.673	1.00 52.94	В	C
	ATOM	4018	CB		B 387	3.430	27.924	52.898	1.00 52.84	В	C
	ATOM	4019 4020	OG C		B 387 B 387	4.439	26.960 26.788	52.630 51.181	1.00 53.68 1.00 53.55	B	o c
	ATOM	4021	ŏ		B 387	2.221	25.788	51.101	1.00 56.01	В	Ö
50	ATOM	4022		SER		1.426	26.735	50.087	1.00 52.55	В	ŏ
	TER	4023			B 387						
	ATOM	4024	C1	FRA .		21.364	83.849	79.751	1.00 28.06	Z	C
	ATOM	4025	C2	FRA :		21.204	82.482	80.488	1.00 28.48	z z	C
55	ATOM	4026	C3 C4	FRA .		20.089 20.171	81.594 81.530	79.848 78.286	1.00 28.20 1.00 29.96	Z	c
55	ATOM	4028	C5	FRA		20.171	82.931	77.637	1.00 26.40	z	č
	ATOM	4029	N6	FRA		21.562	83.678	78.268	1.00 26.70	ž	N
	ATOM	4030	C7	FRA		21.844	85.007	77.590	1.00 26.79	Z	С
	ATOM	4031	C8	FRA		22.091	84.946	76.062	1.00 22.84	Z	C
60	ATOM	4032	C9	FRA		21.703	86.217	75.301	1.00 22.28	Z	C
	ATOM ATOM	4033 4034		FRA		22.186 22.294	86.127	73.930	1.00 21.29 1.00 20.50	z z	0
	ATOM	4034		FRA		22.781	87.227 87.073	73.066 71.728	1.00 20.50	Z	C
	ATOM	4036	C13	FRA	z 1	22.881	88.197	70.870	1.00 17.71	z	C
65	ATOM	4037	C14	FRA	z 1	22.506	89.483	71.312	1.00 15.27	Z	C
	ATOM	4038	C15	FRA	z 1	22.005	89.651	72.695	1.00 16.51	z	C
	ATOM	4039		FRA		21.911	88.516	73.537	1.00 18.78	z	C
	ATOM	4040 4041		FRA		21.634 21.733	90.872 91.911	73.162 72.347	1.00 18.92 1.00 15.67	z z	N C
70	ATOM	4041		FRA		22.169	91.911	71.088	1.00 15.67	z	N
	ATOM	4043		FRA		22.560	90.693	70.539	1.00 16.78	z	C
	ATOM	4044		FRA		23.025	90.704	69.148	1.00 16.94	z	N

	ATOM	4045	ann	FRA	_	1	22 221	-101-	CO 100	1 00 10 00	7.	
	ATOM	4045		FRA		1	23.001 24.061	91.757 91.923	68.180 67.246	1.00 18.96 1.00 17.20	2.	C
	ATOM	4045		FRA		1	24.061	92.933	66.367	1.00 17.20	2 2	N
	ATOM	4047			Z	1	24.042	92.933	66.394	1.00 19.55	Z	C
5	ATOM	4048	N26		Z	1	22.992	93.788	67.214	1.00 18.00	Z	N
,	ATOM	4050	C27	FRA		1	21.935	92.724	68.097	1.00 17.17	Z	. C
	ATOM	4051	N28		z	1	23.043	94.876	65.467	1.00 18.78	Z	N
	ATOM	4051	C29		Z	1	23.696	95.214		1.00 22.15	Z	C
	ATOM	4052		FRA		1			64.346		Z	c
10	ATOM	4054		FRA		1	23.352	96.585	63.786	1.00 19.36	2	
10		4054					22.405	97.470	64.411	1.00 17.69		C
	ATOM			FRA		1	22.122	98.742	63.860	1.00 20.12	Z	C
	ATOM	4056		FRA		1	22.776	99.153	62.676	1.00 17.24	Z	C
	ATOM	4057		FRA		1	23.710	98.303	62.042	1.00 17.77	Z	c
10	ATOM	4058		FRA		1	23.998	97.035	62.589	1.00 17.80	Z	c
15	ATOM	4059		FRA		1	24.531	94.448	63.824	1.00 21.83	Z	0
	MOTA	4060	037			1	23.170	85.827	71.240	1.00 20.79	Z	0
	ATOM	4061		FRA		1	22.679	85.375	69.951	1.00 26.55	Z	C
	ATOM	4062	039	FRA		1	23.466	84.677	75.820	1.00 24.51	Z	0
	TER	4063		PRA		1						
20	ATOM	4064	C1	FRA		1	1.515	35.986	27.679	1.00 36.52	Y	С
	ATOM	4065	C2	FRA		1	0.608	36.976	26.867	1.00 37.59	Y	C
	ATOM	4066	C3	FRA		1	-0.401	36.230	25.961	1.00 36.15	Y	С
	ATOM	4067	C4	FRA		1	0.319	35.193	25.054	1.00 37.83	Y	C
	ATOM	4068	C5	FRA		1	1.177	34.183	25.879	1.00 36.12	Y	C
25	ATOM	4069	N6	FRA		1	2.132	34.827	26.897	1.00 36.16	Y	N
	ATOM	4070	C7	FRA		1	3.479	35.234	26.297	1.00 37.30	Y	C
	ATOM	4071	C8	FRA		1	4.332	34.189	25.489	1.00 32.04	Y	C
	ATOM	4072	C9	FRA		1	4.647	32.852	26.202	1.00 29.29	Y	C
	ATOM	4073		FRA		1	6.097	32.795	26.275	1.00 25.58	Y	0
30	ATOM	4074		FRA		1	6.903	31.673	26.442	1.00 20.22	Y	С
	ATOM	4075		FRA		1	8.327	31.834	26.469	1.00 19.90	Y	С
	ATOM	4076		FRA		1	9.170	30.706	26.629	1.00 18.27	Y	C
	ATOM	4077		FRA		1	8.622	29.412	26.769	1.00 16.62	Y	C
	ATOM	4078	C15	FRA		1	7.143	29.247	26.749	1.00 16.07	Y	C
35	ATOM	4079		FRA		1	6.320	30.391	26.580	1.00 17.70	Y	C
	ATOM	4080	N17	PRA		1	6.583	28.029	26.887	1.00 17.71	Y	N
	ATOM	4081		FRA		1	7.389	26.981	27.040	1.00 17.21	Y	C
	ATOM	4082		FRA		1	8.725	27.007	27.067	1.00 17.12	Y	N
	ATOM	4083		FRA		1	9.371	28.193	26.934	1.00 17.89	Y	С
40	ATOM	4084		FRA		1	10.845	28.199	26.966	1.00 19.44	Y	N
	ATOM	4085		FRA		1	11.804	27.160	27.225	1.00 17.92	Y	C
	ATOM	4086		FRA		1	13.046	27.089	26.514	1.00 17.84	Y	C
	ATOM	4087		FRA		1	13.927	26.091	26.750	1.00 17.67	Y	N
	ATOM	4088	C25	FRA		1	13.591	25.172	27.677	1.00 19.86	Y	С
45	ATOM	4089		FRA		1	12.465	25.164	28.390	1.00 22.22	Y	N
	ATOM	4090		FRA		1	11.584	26.130	28.180	1.00 20.19	Y	C
	ATOM	4091		FRA		1	14.520	24.102	27.878	1.00 21.17	Y	N
	ATOM	4092		FRA		1	15.769	23.800	27.502	1.00 20.01	Y	C
	ATOM	4093		FRA		1	16.310	22.465	27.980	1.00 19.29	Y	C
50	ATOM	4094		FRA		1	15.545	21.551	28.783	1.00 19.61	Y	C
	ATOM	4095		FRA		1	16.081	20.315	29.195	1.00 21.23	Y	C
	ATOM	4096		FRA		1	17.394	19.964	28.819	1.00 18.14	Y	C
	ATOM	4097		FRA		1	18.172	20.843	28.033	1.00 19.61	Y	С
	ATOM	4098		FRA		1	17.642	22.083	27.612	1.00 19.21	Y	C
55	ATOM	4099	036	FRA	Y	1	16.421	24.575	26.797	1.00 19.90	Y	0
	ATOM	4100		FRA		1	8.904	33.109	26.339	1.00 21.63	Y	0
	ATOM	4101		FRA		1	10.186	33.273	25.678	1.00 23.16	Y	С
	ATOM	4102	039	FRA		1	3.746	33.908	24.230	1.00 36.52	Y	0
60	TER	4103		FRA		1						
	ATOM	4104	0	HOH		1	-2.816	80.929	50.812	1.00 19.03	E	0
	ATOM	4105	0	HOH		2	3.978	72.365	54.056	1.00 19.03	E	0
	ATOM	4106	0	HOH		3	13.505	98.252	72.880	1.00 19.36	E	0
	ATOM	4107	0	HOH		4	28.293	104.582	83.681	1.00 21.47	E	0
65	ATOM	4108	0	HOH		6	6.360	44.178	47.881	1.00 23.42	E	0
	ATOM	4109	0	HOH		7	1.770	73.865	68.162	1.00 20.46	E	0
	ATOM	4110	0	HOH		8	8.297	17.524	35.431	1.00 28.17	E	0
	MOTA	4111	0	HOH		9	4.373	82.422	53.549	1.00 66.83	E	0
	ATOM	4112	0	HOH		10	9.876	77.587	53.891	1.00 15.33	E	0
70	MOTA	4113	0	HOH		11	13.114	23.318	30.599	1.00 23.68	E	0
	ATOM	4114	0	HOH		12	7.067	14.767	42.081	1.00 41.33	E	0
	MOTA	4115	0	HOH	В	13	15.665	28.507	29.364	1.00 35.38	E	0

						-102-				
	ATOM	4116 4117	0	HOH E	14 15	8.724 81.834 21.092 27.236	51.911	1.00 15.54 1.00 29.72	E	0
	ATOM	4118	o	HOH B	16	4.235 23.958	10.152	1.00 29.72	E	0
_	ATOM	4119	0	HOH E	17	21.990 41.088	42.974	1.00 32.56	E	ō
5	ATOM	4120	0	HOH E	18	20.666 46.477	48.657	1.00 22.11	E	0
	ATOM	4121 4122	0	HOH E	19 20	12.394 30.572 24.458 88.275	26.200 67.914	1.00 25.85 1.00 18.95	E	0
	ATOM	4123	ő	HOH E	21	16.023 94.041	76.489	1.00 18.64	E	ö
	ATOM	4124	O	HOH E	22	-3.046 75.441	65.884	1.00 19.92	E	ō
10	ATOM	4125 4126	0	HOH E	24 25	13.742 101.239	70.093	1.00 20.42	E	0
	ATOM	4125	0	HOH E	26	2.139 79.403 -0.923 97.738	76.859 56.694	1.00 24.59 1.00 26.97	E	0
	ATOM	4128	ŏ	HOH E	27	27.493 25.824	48.659	1.00 25.58	E	ő
	ATOM	4129	0	HOH E	28	-3.060 85.100	45.284	1.00 28.40	В	0
15	ATOM	4130	0	HOH E	29	2.126 21.471	26.630	1.00 18.24	E	0
	ATOM	4131 4132	0	HOH E	30 31	19.055 98.237 5.015 20.070	66.551 34.897	1.00 26.93 1.00 27.21	E	0
	ATOM	4133	ŏ	HOH E	32	20.699 97.163	78.060	1.00 20.06	E	ő
	ATOM	4134	0	HOH E	33	19.905 95.504	66.214	1.00 16.74	E	0
20	ATOM	4135 4136	0	HOH E	34 35	26.799 36.524	56.357	1.00 23.12	E	0
	ATOM	4137	0	HOH E	36	7.281 42.459 -5.229 82.177	52.886 76.134	1.00 27.29 1.00 17.35	E	0
	ATOM	4138	0	HOH E	37	16.156 81.681	74.210	1.00 33.58	E	Ö
	ATOM	4139	0	HOH E	38	17.171 26.456	35.298	1.00 26.63	E	0
25	ATOM	4140 4141	0	HOH E	41	10.220 96.211	76.240	1.00 36.39	E	0
	ATOM	4142	0	HOH E	43	21.575 87.342 -2.344 82.211	80.619 46.311	1.00 26.03 1.00 33.39	E	0
	ATOM	4143	ō	HOH E	44	1.411 102.153	63.920	1.00 40.99	E	o
20	ATOM	4144	0	HOH E	45	22.412 37.472	55.894	1.00 36.08	E	0
30	ATOM	4145 4146	0	HOH E	46	2.300 24.457 13.621 22.599	31.665	1.00 23.22 1.00 23.98	E	0
	ATOM	4147	ŏ	HOH E	48	15.021 22.333	55.761	1.00 28.43	E	0
	ATOM	4148	0	HOH E	49	14.580 93.564	78.622	1.00 24.96	E	0
35	ATOM	4149	0	HOH E	50	26.890 18.450	12.611	1.00 42.82	E	0
33	ATOM	4150 4151	0	HOH E	51 52	9.227 107.514 34.558 108.086	67.012 67.299	1.00 41.46 1.00 37.65	E	0
	ATOM	4152	ŏ	HOH E	53	10.050 90.871	55.783	1.00 29.24	E	ö
	ATOM	4153	0	HOH E	54	7.944 16.482	49.236	1.00 41.77	E	0
40	ATOM ATOM	4154 4155	0	HOH E	55 56	13.318 100.169 7.437 71.694	53.864 56.237	1.00 42.27	Ε.	0
40	ATOM	4156	ö	HOH E	57		25.399	1.00 34.69	E	0
	ATOM	4157	0	HOH E	58		70.952	1.00 40.32	E	ŏ
	ATOM	4158	0	HOH E	59	16.826 72.690	51.895	1.00 39.22	E	0
45	ATOM	4159 4160	0	HOH E	60 61	26.960 20.330 24.484 34.166	32.431 17.080	1.00 46.00 1.00 57.71	E	0
75	ATOM	4161	ŏ	HOH E	62		24.722	1.00 36.63	E	0
	ATOM	4162	0	HOH E	63	2.410 82.045	76.883	1.00 31.15	E	ō
	ATOM	4163	0	HOH E	64	20.509 17.863	8.881	1.00 34.06	E	0
50	ATOM	4164 4165	0	HOH E	65 66		47.676 72.560	1.00 36.58 1.00 35.02	E	0
	ATOM	4166	ŏ	HOH E	67		73.283	1.00 34.26	E	ö
	ATOM	4167	0	HOH E	68	20.674 96.637	81.076	1.00 32.24	E	0
	ATOM ATOM	4168 4169	0	HOH E	69		76.526	1.00 39.65	E	0
55	ATOM	4170	0	HOH E	70 71		50.070 39.187	1.00 41.17 1.00 32.26	E	0
-	ATOM	4171	ŏ	HOH E	72		23.837	1.00 32.20	E	ö
	MOTA	4172	0	HOH E	73	35.386 104.215	87.572	1.00 48.96	E	0
	ATOM	4173 4174	0	HOH E	74 75		63.076	1.00 45.88	E	0
60	ATOM	4175	0	HOH E	76		47.461 66.851	1.00 37.66 1.00 30.87	E	0
	ATOM	4176	ŏ	HOH E	77	11.320 20.363	58.814	1.00 46.67	E	ő
	ATOM	4177	0	HOH E	78	-6.338 85.994	41.967	1.00 51.31	E	0
	ATOM	4178 4179	0	HOH E	79 81	3.655 87.067 7.253 86.756	43.145	1.00 39.38 1.00 59.51	E	0
65	ATOM	4180	Ö	HOH E	82		37.906 47.749	1.00 59.51	E	0
	ATOM	4181	0	HOH B	83	-2.313 31.734	47.707	1.00 41.05	В	ŏ
	ATOM	4182	0	HOH E	84	11.459 17.532	33.022	1.00 35.50	E	0
	ATOM	4183 4184	0	HOH E	85 86		41.773 60.380	1.00 28.95 1.00 44.61	E	0
70	ATOM	4185	0	HOH E	87		59.964	1.00 44.61	E	0
	ATOM	4186	ō	HOH E	88	6.136 40.362	59.850	1.00 35.96	E	0
	MOTA	4187	0	HOH E	89	8.854 36.982	12.914	1.00 51.29	В	0

							-103-				
	ATOM	4188	0	HOH E	90	14.894	17.557	10.137	1.00 29.07	E	0
	ATOM	4189	0	HOH E	91	3.598	70.913	41.429	1.00 37.85	E	0
	ATOM	4190	0	HOH E	92	15.660	96.593	64.706	1.00 34.79	E	0
	ATOM	4191	0	HOH E	93	-1.289	22.000	25.700	1.00 53.85	E	0
5	ATOM	4192	0	HOH E	94	18.658	94.873	78.816	1.00 34.79	E	0
	ATOM	4193	0	HOH E	95	24.030	37.111	44.167	1.00 31.33	E	0
	ATOM	4194	0	HOH E	96	24.327	108.825	70.586	1.00 43.44	E	0
	MOTA	4195	0	HOH E	97	17.453	29.940	39.065	1.00 62.04	E	0
	ATOM	4196	0	HOH E	98	-10.095	77.380	58.416	1.00 32.83	E	0
10	ATOM	4197	0	HOH E	99	1.372	41.175	43.439	1.00 30.57	E	0
	ATOM	4198	0	HOH E	100	13.220	40.977	61.050	1.00 25.13	E	0
	ATOM	4199	0	HOH E	101	20.635	23.766	29.311	1.00 36.67	E	0
	ATOM	4200	0	HOH E	102	6.907	103.740	69.211	1.00 39.48	E	0
	ATOM	4201	0	HOH E	103	29.965	20.328	27.392	1.00 35.16	E	0
15	ATOM	4202	0	HOH E	104	-5.202	80.206	74.097	1.00 29.87	E	0
	ATOM	4203	0	HOH E	105	-0.936	62.297	61.894	1.00 42.93	E	0
	ATOM	4204	0	HOH E	106	36.982	102.874	54.415	1.00 36.76	E	0
	ATOM	4205	0	HOH E	107	5.889	102.017	53.094	1.00 63.79	E	0
	ATOM	4206	0	HOH E	108	39.219	43.505	52.395	1.00 38.65	E	0
20	mpp	4207		HOH IS	100						

-104-

The shape of the ATP binding pocket is defined by the atomic coordinates of the atoms in the amino-acid residues in Tables 1 and 2. Table 1 lists the atomic coordinates for [T287D] Aurora A(122-396) catalytic domain, together with the AMP-PNP molecule, in Protein Data Bank (PDB) format, as determined from the first crystalline form. Table 2-lists the atomic coordinates for the two independent molecules of the GSHM-[T287D]Aurora A (122-400) catalytic domain, together with the inhibitor of formula II, in PDB format, as determined from the second crystalline form. The atomic coordinates are listed in those lines that begin with the code ATOM or HETATM, one atom per line. Following the code are: the unique atom number; the atom name; the amino acid residue name; the protein chain identifier; the amino acid residue number; the atomic coordinates x, y, and z in orthogonal Angstrom space; the atomic occupancy factor; the atomic temperature factor; the chain identifier; and the atom type. The atomic coordinates of the ATP analogue AMP-PNP carry the residue name of-ANP. Solvent water molecules carry the residue name of HOH, and a citrate and a bound phosphate derived from the crystallisation buffer carry the residue name of FRA. In the inhibitor complex the inhibitor molecules carry the residue name of FRA.

It is possible to reproduce the shape of the [T287D]Aurora A active site binding pocket through carrying out similar structure determinations with minor variations in the experimental conditions (including variations in construct such as mutants, variants and homologues, variations in crystallisation conditions, crystal form, trial model used in 20 molecular replacement, etc.). Different experiments may give rise to apparently different coordinates, but those in the art will realise that two apparently different sets of coordinates for the same or similar proteins can be shown to be equivalent by superposition of the molecules. For example, the coordinates in Tables 1 and 2 are different numerically. But following superposition they can be seen to describe the same molecule. It will be appreciated that, 25 according to accepted practice, the atomic coordinates may vary within certain limits due to experimental variation. Such variation includes standard experimental error (coordinates determined for the same construct may vary somewhat, for example within 0.3 Å) and other variation (for example, coordinates of Aurora mutants, variants, or homologues). The coordinates of the active site ATP binding site may also differ upon introduction of a different 30 small molecule inhibitor, where flexible portions of the binding site adopt a new conformation specific to a type of inhibitor. For example, following superposition, the protein coordinates in Table 1 are seen to be marginally different to those in Table 2, as a result of flexible portions of the protein being influenced by the presence of a different inhibitor. This constitutes a

-105-

modification of the active site ATP binding site rather than the creation of a new site. Those in the art will realise that kinases in general have flexible active sites, and adopt a number of biologically relevant conformations related to the state of catalytic activation. Therefore, for the purposes of differentiating the shape of the active site ATP-binding pocket from that in 5 other kinases, the binding pocket is best defined by a subset of amino acids that are least affected by flexible protein responses to inhibitor binding. Thus, a protein can be said to have the Aurora active site described here if, following superposition, the positions of all atoms in the active site residues in set B, i.e. Arg136, Leu138, Glv139, Val146, Ala159, Lvs161, Leu163, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, 10 Leu214, Gly215, Thr216, Arg219, Glu259, Asn260 and Leu262 or their equivalents, are within a root mean square deviation of 1.0 Å of the coordinates of these amino acid residues given in Tables 1 and 2. An equivalent residue is an amino acid residue in any Aurora mutant, variant, or homologue that occurs at one of the amino acid sequence positions in Tables 1 or 2 - if the residue is not identical, only the N, Ca, CB, C, O atoms may be sensibly included in 15 the rmsd calculation. It is also understood that if equivalent residues are not present in a particular variant or homologue, then they are omitted from the calculation of the average distance

The criterion of 1.0 Å is intended to be large enough to allow the types of variations described above, yet small enough to discriminate between the active sites of Aurora kinases and other kinases. That this criterion is reasonable is illustrated in Table 3, which compares [T287D]Aurora A to one of the most closely related kinases, PKA.

			1atp	113r	1bx6	1apm	1ydt	1cmk
1-2	0.85	1-PKA	1.32	1.32	1.29	1.24	1.28	1.17
1 - 3	0.67	2-PKA	1.19	1.14	1.08	1.13	1.13	1.13
2 - 3	0.42	3-PKA	1.14	1.08	1.09	1.08	1.10	1.21

Table 3: rms deviations in Å between all atoms of set B amino acids in the active site.

25 The top row refers to the PDB codes for 6 entries of a different kinase, protein kinase A (PKA). The bold numbers refer to the Tables 1 and 2 which contain Aurora coordinates. Thus, when independent structure determinations of Aurora are compared (1-2, 1-3, 2-3) the rmsd is

-106-

less than 1 Å, whereas when Aurora is compared to PKA (6 independent structures) the rmsd is greater than 1 Å.

Thus, according to a further aspect of the invention, we provide the shape of the active 5 site ATP binding pocket in Aurora protein kinase as defined by the atomic coordinates given in Tables 1 and 2 or by equivalent coordinates. Equivalent coordinates are those for which the subset of least flexible residues (set B) have atomic positions on average within 1.0 Å of those in the Aurora active site ATP binding pocket as defined by the coordinates in Tables 1 and 2.

According to a further aspect of the invention we provide a method to determine or

design the three-dimensional structure of a crystal form of Aurora (including Aurora A

homologues, variants, mutants, and inhibitor complexes) by using a particular Aurora A

catalytic domain structure. The atomic co-ordinates of an Aurora A crystal may be used to

model the structure of a second Aurora crystal by difference Fourier or molecular replacement

methods

The crystal structure of the Aurora A kinase catalytic domain described herein can be used to model the three-dimensional structures of other Aurora kinases. Furthermore, alternative methods of determining three-dimensional structure that do not rely on X-ray diffraction techniques and thus do not require crystallization of the protein, such as NMR techniques, are simplified if a model of the structure is available for refinement using the additional data gathered by the alternative technique. Thus, definition of the three-dimensional structure of the catalytic domain of Aurora A kinase enables one of skill in the art to determine the structure of the catalytic domains of other Aurora kinases.

Knowledge of the three-dimensional structure of the catalytic domain of Aurora A
kinase provides a means for investigating the mechanism of action of the protein and tools for
identifying inhibitors of its function. Knowledge of the three-dimensional structure of the
catalytic domain of Aurora A kinase allows one to design molecules capable of binding
thereto, including molecules which are capable of inhibiting (partially or completely) the
activity of Aurora A kinase.

Illustrative crystalline forms of polypeptides of this invention having various
physicochemical characteristics are disclosed herein. Preferred crystalline forms invention are
capable of diffracting x-rays to a resolution of better than about 3.5 Å, and more preferably to
a resolution of 3.0 Å or better, and even more preferably to a resolution of 2.2 Å or better, and
are useful for determining the three-dimensional structure of the material.

-107-

Crystalline compositions of this invention specifically include those in which the crystals comprise Aurora kinase family proteins characterized by the structural coordinates set forth in any of the accompanying tables or characterized by coordinates having a root mean square deviation therefrom, with respect to backbone atoms of amino acids given in the 5 Tables, of 1.5 Å or less. Crystalline compositions of this invention also include those in which the crystals comprise Aurora kinase family proteins characterized by having a binding site defined by the x,y,z-coordinates of atoms in the set of amino acid residues (set A) given by the list Arg136, Leu138, Glv139, Lvs140, Glv141, Val146, Lvs161, Leu163, Val177, Glu180, Val181, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, 10 Pro213, Leu214, Gly215, Thr216, Arg219, Glu259, Asn260, Leu262, Ala272, Asp273, Phe274, Gly275, Trp276, Ser277, Val278, and His279, the atomic coordinates being listed in Tables 1 and 2. Further, crystalline forms of polypeptides of this invention also include those in which the crystals comprise Aurora kinase family proteins in which the binding site is defined by the x,y,z-coordinates of atoms in the set of amino acid residues (set B) given by the 15 list Arg136, Leu138, Gly139, Va1146, Ala159, Lys161, Leu163, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215, Thr216, Arg219, Glu259, Asn260 and Leu262 or their equivalent, are within a root mean square deviation of 1.0 Å of the coordinates of these amino acid residues given in Tables 1 and 2.

Structural coordinates of a crystalline composition of this invention may be stored in a
machine-readable form on a machine-readable storage medium, such as a computer hard
drive, diskette, DAT tape, for display as a three-dimensional shape or for other uses involving
computer-assisted manipulation of, or computation based on, the structural coordinates or the
three-dimensional structures they define. For example, data defining the three dimensional
structure of a protein of the Aurora kinase family, or portions or structurally similar

25 homologues of such proteins, may be stored in a machine-readable storage medium and
displayed as a three-dimensional representation of the protein structure, typically using a
computer capable of reading the data from said storage medium and programmed with
instructions for creating the representation from such data. This invention thus encompasses a
machine, such as a computer, having a memory which contains data representing the structural
coordinates of a crystalline composition of this invention, such as the coordinates set forth in
Tables 1 and 2, together with additional optional data and instructions for manipulating such
data. Such data may be used for a variety of purposes, such as the elucidation of other related
structures and drug discovery.

-108-

For example, a first set of such machine readable data may be combined with a second set of machine-readable data using a machine programmed with instructions for using the first data set and the second data set to determine at least a portion of the coordinates corresponding to the second set of machine-readable data. For instance, the first set of data 5 may comprise a Fourier transform of at least a portion of the coordinates for Aurora kinase proteins set forth in Tables 1 and 2, while the second data set may comprise X-ray diffraction data of a molecule or molecular complex.

More specifically, one of the objects of this invention is to provide three-dimensional structural information on new complexes of Aurora kinase family members (e.g., complexed 10 with an ATP analogue or an inhibitor, such as a synthetic inhibitor), new Aurora kinase family members and variants of any of the foregoing. The structural coordinates of a crystalline composition of this invention, or portions thereof, can be used to solve, e.g. by molecular replacement, the three dimensional structure of a crystalline form of such a polypeptide or polypeptide complex. Doing so involves obtaining x-ray diffraction data for crystals of the 15 polypeptide or polypeptide complex (e.g., in complex with an ATP analogue or an inhibitor, such as a synthetic inhibitor) for which one wishes to determine the three dimensional structure. The three-dimensional structure of that polypeptide or complex is determined by analyzing the x-ray diffraction data using molecular replacement techniques with reference to the structural coordinates provided. For example, molecular replacement can use a molecule 20 having a known structure as a starting point to model the structure of an unknown crystalline sample. This technique is based on the principle that two molecules which have similar structures, orientations and positions in the unit cell diffract similarly. The term "molecular replacement" refers to a method that involves generating a preliminary model of a crystal whose atomic coordinates are not known, by orienting and positioning a related molecule 25 whose atomic coordinates are known. Phases are then calculated from this model and combined with observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. Molecular replacement involves positioning the known structure in the unit cell in the same location and orientation as the unknown structure. Once positioned, the atoms of the known structure in the unit cell are used to calculate the structure 30 factors that would result from a hypothetical diffraction experiment. This involves rotating the known structure in the six dimensions (three angular and three spatial dimensions) until alignment of the known structure with the experimental data is achieved. This approximate structure can be refined to yield a more accurate and often higher resolution structure using

-109-

various refinement techniques. For instance, the resultant model for the structure defined by the experimental data may be subjected to rigid body refinement in which the model is subjected to limited additional rotation in the six dimensions yielding positioning shifts of under about 5%. The refined model may then be further refined using other known 5 refinement methods.

For example, one may use molecular replacement to exploit a set of coordinates such as set forth in Table 1 or Table 2 to determine the structure of the catalytic domain of Aurora kinase in complex with other than ATP-PNP or the inhibitor of formula II.

The present invention also relates to designing and, optionally producing, a homologue 10 of Aurora kinase, such as a homologue of Aurora kinase A, that mimics the three-dimensional structure of the Aurora kinase. The method comprises:

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- (i) determining the three-dimensional coordinates of atoms of an Aurora kinase;
- (ii) providing a computer having a memory means, a data input means, a visual display means, said memory means containing three-dimensional molecular simulation software operable to retrieve co-ordinate data from said memory means and to display a three-dimensional representation of a molecule on said visual display means and being operable to produce a modified three-dimensional homologue representation responsive to operator-selected changes to the structure of the Aurora kinase and to display the three-dimensional representation of the modified three-dimensional homologue;
- (iii) inputting three-dimensional co-ordinate data of atoms of Aurora kinase into the computer and storing said data in the memory means;
- inputting into the data input means of said computer at least one operatorselected change in structure of the Aurora kinase;
- (v) executing said molecular simulation software to produce a modified threedimensional molecular representation of the homologue structure;
- (vi) displaying the three-dimensional representation of the homologue on said visual display means, whereby changes in three-dimensional structure of the Aurora kinase resulting from changes on structure can be visually monitored;
- (vii) repeating steps (iv) through (vi) to produce a multiplicity of homologues; and
 - (viii) selecting a homologue structure represented by a three-dimensional representation wherein the three-dimensional configuration and spatial arrangements of the kinase catalytic domain remain substantially preserved,

-110-

thereby producing a homologue of Aurora kinase that mimics the threedimensional structure of the Aurora kinase.

The present invention also relates to a method of producing a modulator of Aurora kinase (particularly inhibitors), such as a modulator of Aurora kinase A. The method 5 comprises identifying a compound or molecule or designing a compound or molecule that fits into the active site ATP binding pocket of the Aurora kinase, wherein the ATP binding pocket is defined by (a) Arg136, Leu138, Gly139, Lys140, Gly141, Val146, Lys161, Leu163, Val177, Glu180, Val181, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215, Thr216, Arg219, Glu259, Asn260, Leu262, Ala272, Asp273, 10 Phe274, Gly275, Trp276, Sez277, Val278, and His279, the atomic coordinates being listed in Tables 1 and 2 or (b) the x,y,z- coordinates of atoms in the set of amino acid residues (set B) given by the list Arg136, Leu138, Gly139, Val146, Ala159, Lys161, Leu163, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215, Thr216, Arg219, Glu259, Asn260 and Leu262, each having coordinates as described in

15 Tables 1 and 2, thereby producing a modulator of Aurora kinase.

Another object of the invention is to provide a method for determining the threedimensional structure of the catalytic domain of an Aurora kinase protein, or the catalytic domain of an Aurora kinase protein in complex with an inhibitor, using homology modeling techniques and structural coordinates for a composition of this invention. Homology 20 modeling involves constructing a model of an unknown structure using structural coordinates of one or more related proteins, protein domains and/or subdomains. Homology modeling may be conducted by fitting common or homologous portions of the protein or peptide whose three dimensional structure is to be solved to the three dimensional structure of homologous structural elements. This approach can be used to rebuild part or all of a three dimensional 25 structure with replacement of amino acids (or other components) by those of the related structure to be solved. For example, using the structural coordinates of the catalytic domain of an Aurora kinase in complex with AMP-PNP or the inhibitor of formula II, it is possible to determine the three dimensional structure of the catalytic domain of another Aurora kinase protein through the use of homology modeling. Those coordinates may be stored, displayed, 30 manipulated and otherwise used in like fashion as the Aurora kinase coordinates of Tables 1-2.

Thus, crystalline compositions of this invention provide a starting material for use in solving the three-dimensional structure of other Aurora kinase polypeptides.

-111-

By way of further example, the structure defined by the machine readable data may be computationally evaluated for its ability to associate with various chemical entities. The term "chemical entity", as used herein, refers to chemical compounds, complexes of at least two chemical compounds, and fragments of such compounds or complexes.

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For instance, a first set of machine-readable data defining the three-dimensional structure of an Aurora kinase family protein, or a portion or complex thereof, is combined with a second set of machine-readable data defining the structure of a chemical entity or moiety of interest using a machine programmed with instructions for evaluating the ability of the chemical entity or moiety to associate with the Aurora kinase family protein or portion or 10 complex thereof and/or the location and/or orientation of such association. Such methods provide insight into the location, orientation and energetics of association of the Aurora kinase family protein with such chemical entities. Chemical entities that associate or interact with an Aurora kinase may inhibit its interaction with naturally occurring ligands for the protein and may inhibit biological functions mediated by such interaction. Such chemical entities are drug 15 candidates.

The protein structure encoded by the data may be displayed in a graphical format permitting visual inspection of the structure, as well as visual inspection of the structure's association with chemical entities. Alternatively, more quantitative or computational methods may be used. For example, one method of this invention for evaluating the ability of a 20 chemical entity to associate with any of the molecules or molecular complexes set forth herein comprises the steps of: a) employing computational means to perform a fitting operation between the chemical entity and a binding pocket or other surface feature of the molecule or molecular complex; and b) analyzing the results of the fitting operation to quantify the association between the chemical entity and the binding pocket.

This invention further provides for the use of the structural coordinates of a crystalline composition of this invention, or portions thereof, to identify reactive amino acids, such as cysteine residues, within the three-dimensional structure, such as within or adjacent to the catalytic domain; to generate and visualize a molecular surface, such as a water-accessible surface or a surface comprising the space-filling van der Waals surface of all atoms; to 30 calculate and visualize the size and shape of surface features of the protein or complex, e.g., ligand binding pockets; to locate potential H-bond donors and acceptors within the threedimensional structure, preferably within or adjacent to a ligand binding site; to calculate regions of hydrophobicity and hydrophilicity within the three-dimensional structure,

-112-

preferably within or adjacent to a ligand binding site; and to calculate and visualize regions on or adjacent to the protein surface of favorable interaction energies with respect to selected functional groups of interest (e.g. amino, hydroxyl, carboxyl, methylene, alkyl, alkenyl, aromatic carbon, aromatic rings, heteroaromatic rings, substituted and unsubstituted fluoro and diffuorophosphonates; etc.). One may use the foregoing approaches for characterizing the protein and its interactions with moieties of potential ligands to design or select compounds capable of specific covalent attachment to reactive amino acids (e.g., cysteine) and to design or select compounds of complementary characteristics (e.g., size, shape, charge, hydrophobicity/hydrophilicity, ability to participate in hydrogen bonding, etc.) to surface features of the protein, a set of which may be preselected. Using the structural coordinates, one may also predict or calculate the orientation, binding constant or relative affinity of a given ligand to the protein in the complexed state, and use that information to design or select compounds of improved affinity.

In such cases, the structural coordinates of the Aurora kinase family protein, or portion or complex thereof, are entered in machine readable form into a machine programmed with instructions for carrying out the desired operation and containing any necessary additional data (e.g. data defining structural and/or functional characteristics of a potential ligand or moiety thereof, defining molecular characteristics of the various amino acids).

One method of this invention provides for selecting from a database of chemical structures a molecular compound capable of binding to an Aurora kinase family protein (e.g., coordinates defining the three dimensional structure of an Aurora kinase family protein or a portion thereof). Points associated with the three dimensional structure (structural coordinates) of a crystalline form of Aurora A kinase catalytic domain are characterized with respect to the favorability of interactions with one or more functional groups. A database of chemical structures is then searched for candidate compounds containing one or more functional groups disposed for favorable interaction with the protein based on the prior characterization. Compounds having structures which best fit the points of favorable interaction with the three dimensional structure are thus identified.

It is often preferred, although not required, that such searching be conducted with the aid of a computer. In that case a first set of machine-readable data defining the three-dimensional structure of an Aurora kinase family protein, or a portion or complex thereof, is combined with a second set of machine readable data defining one or more moieties or

-113-

functional groups of interest, using a machine programmed with instructions for identifying preferred locations for favorable interaction between the functional group(s) and atoms of the protein. A third set of data, which defines the location(s) of favorable interaction between protein and functional group(s) is generated. The third set of data is then combined with a 5 fourth set of data defining the three-dimensional structures of one or more chemical entities using a machine programmed with instructions for identifying chemical entities containing functional groups to best fit the locations of their respective favorable interaction with the protein.

Compounds of the structures selected or designed by any of the foregoing means may

be tested for their ability to bind to an Aurora kinase family protein, inhibit the binding of an

Aurora kinase family protein to a natural or non-natural ligand therefor, and/or inhibit a

biological function mediated by an Aurora kinase family member.

The new crystal may be a crystal of a homologue, variant, mutant, or inhibitor complex of Aurora. The shape of the Aurora active site binding pocket in the new crystal model is an equivalent shape to that of the first. The active site binding pocket of the original Aurora A crystal is defined by the amino acid residues of set A and their atomic coordinates as given in Tables 1 and 2. Equivalent shape is defined as having an rmsd of less than 1 Å upon superposition of the subset of least flexible amino acid residues (set B).

Thus, the invention provides a method to determine or design the three dimensional
structure of a crystal form of Aurora by difference Fourier or Molecular Replacement, using
the coordinates (Tables 1 and 2) of an Aurora A crystal to model the structure of a new Aurora
crystal wherein the active site ATP binding region is equivalent to that in the first crystal. The
method may be carried out as follows. An Aurora protein (wild type, mutant, variant or
homologue) is purified and crystallised as a pure protein or in complex with an inhibitor
compound. This crystal may have the same crystal form (same protein packing) as one of the
crystal structures defined by Tables 1 and 2, or it may have a different crystal form (different
protein packing). By taking diffraction measurements of the crystal and using the atomic
coordinates in Tables 1 or 2 (or equivalent coordinates), it is possible to work out the structure
of the crystal by the known methods of difference Fourier (same packing) or molecular
replacement (different packing). This invention covers the use in drug design of the active site
ATP binding pocket in any new crystal since this will be equivalent to that in the original
crystal.

-114-

The invention further provides Aurora A proteins (including homologues, variants and mutants) designed by the above method. The Aurora A proteins may have identical properties to wild type Aurora A or may have one or more different properties compared to wild type Aurora A.

According to a further aspect of the invention, we provide a method to select or design chemical modulators (preferably inhibitors) of Aurora by using the Aurora A catalytic domain structure (including that of homologues, variants, mutants, and inhibitor complexes) and the shape of the active site ATP binding pocket (or an equivalent shape as previously defined). Information from the three dimensional atomic coordinates of the AMP-PNP molecule and its spatial orientation in relation to the three dimensional atomic coordinates of the Aurora A catalytic domain is used as a tool to design Aurora modulators (preferably inhibitors). In addition, information from the three dimensional atomic coordinates of the inhibitor molecule of formula II and its spatial orientation in relation to the three dimensional atomic coordinates of the Aurora A catalytic domain is used as tool to design Aurora modulators (preferably inhibitors). Small-molecule modulators of Aurora may be selected or designed to fit into the shape of the active site binding pocket.

Knowledge of the structural determinants that account for the difference in substrate specificity between Aurora A and other kinases, such as PKA, provides a foundation for the design of highly specific modulators of the Aurora A enzyme. Structural differences at the 20 ATP binding pocket between Aurora and other kinases (defined by differences in the atomic coordinates of residues in the ATP pocket) may be used to design selective Aurora A modulators.

According to a further aspect of the invention, use of the coordinates of the Aurora A catalytic domain (Tables 1 and 2) to locate other pockets for interaction by small molecule modulators that affect Aurora activity is claimed. Such pockets may overlap with the active site ATP binding pocket or be completely independent. The three-dimensional structure of Aurora A kinase is an essential tool in the discovery of any such pockets that provide an alternative for modulator interaction to the active site ATP binding pocket.

As described above, the Aurora A crystal structure may be used in the rational design
of drugs which modulate (preferably inhibit) the action of Aurora. These Aurora modulators
may be used to prevent or treat the undesirable physical and pharmacological consequences of
inappropriate Aurora activity.

-115-

The present invention will now be described with reference to the following nonlimiting Examples.

Definition of Terms

5 In the Description (including the Examples) the following terms are used:

The term "atomic co-ordinates" refers to mathematical co-ordinates corresponding to the positions of every atom derived from mathematical equations related to the diffraction patterns obtained from a monochromatic beam of X-rays illuminating a crystal. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal. Those of skill in the art understand that a set of atomic coordinates determined by X-ray crystallography is not without standard error or experimental variation.

The term "unit cell" refers to the basic building block from which the entire volume of 15 a crystal may be constructed.

The term "space group" refers to the arrangement of symmetry elements within a unit cell.

The term "molecular replacement" refers to a method that involves generating a preliminary model of a crystal whose atomic co-ordinates are not known, by orienting and 20 positioning a related molecule whose atomic co-ordinates are known. Phases are then calculated from this model and combined with observed amplitudes to give an approximate Fourier synthesis of the structure whose co-ordinates are unknown.

Example 1: Production of the kinase catalytic domain of Aurora A

25 Molecular Biology:

In order to obtain a polypeptide (or protein) that can be utilised for determination of the three dimensional (tertiary) structure of Aurora A, DNA encoding Aurora A may be obtained by total gene synthesis or by cloning. This DNA may then be expressed in a suitable expression system to obtain a polypeptide that can be subjected to techniques to determine its three dimensional structure.

In this case, the human Aurora A gene carrying an artificially induced mutation (GAT to ACT in nucleotides 862-864, taking the A of the initial ATG in the open reading frame of the gene to be +1) encoding for a threonine to aspartate (T to D using the single letter amino

-116-

acid code) mutation of amino acid 287 (taking the first amino acid immediately after the initial methionine as amino acid number one) formed the basis of the expression construct used in these studies. This [T287D]Aurora A mutant was a gift of Dr. Jim Bischoff, SUGEN Inc. Since the full length [T287D]Aurora A protein expressed in E.coli was poorly soluble 5 and aggregated on purification, a truncated mutant form was generated. The regions encoding for amino acids 94 to the stop codon of [T287D] Aurora A was amplified using the polymerase chain reaction (PCR). The 5' PCR primer (5'GATCGATCGGATCCACCCAAAAGAGCAAGCAGCCC 3'; SEQ ID NO.: 1) carried a spacer region (to allow efficient cleavage by restriction endonuclease), the BamH1restriction 10 endonuclease recognition sequence and sequence corresponding to the bases 283-301. The 3' primer (5' TGACGCTAGGATCCCCTAAGACTGTTTGCTAGCTGATTC 3'; SEQ ID NO.: 2) carried a spacer region, BamH1 recognition sequence and 3' end of the Aurora A (bases 1189-1212) sequence including the stop codon. PCR products were purified and cloned in to the pCR-Script vector (Stratagene) using the pCR-Script AMP cloning kit (Stratagene. 15 product # 211188) according to manufacturers directions. The pCR-Script vector carrying the [T287D] Aurora A (94-402) sequence was digested with BamH1, the digestion products resolved by agarose gel electrophoresis and the DNA fragment corresponding to the [T287D] Aurora A (94-402) sequence excised and purified using a Qiagen QIAquick kit (Qiagen product #28704). This fragment was then ligated into the vector pTB375NBSE, which had 20 previously been cut with BamH1. (Details of the methods for the assembly of recombinant DNA molecules can be found in standard texts, for example Sambrook et al. 1989, Molecular Cloning - A Laboratory Manual, 2nd Edition, Cold Spring hbor Laboratory Press and Ausubel et al. 1999, Current Protocols in Molecular Biology, John Wiley and Sons Inc). The pTB375NBSE vector is derived from pAT153, which is a mobilization-minus derivative of 25 pBR322. The inserted genes were under the control of a bacteriophage T7 promoter and therefore requires expression of the T7 polymerase in trans for efficient transcription in E.coli. The plasmid encodes tetracyline resistance for selection.

The ligation reactions were transfected in-to TOP10 competent *E.coli* (Invitrogen product #C4040-10) and *E.coli* carrying the pTB375NBSE recombinant vectors identified by their ability to grow on media containing tetracycline. Plasmid DNA was extracted from these bacteria and subjected to digestion with the restriction endonuclease EcoR1 to identify those carrying the [T287D] Aurora A (94-402) sequence. The identity of the insert was then confirmed by dideoxy chain termination DNA sequencing prior to protein expression.

-117-

pTB375NBSE carries the initiation codon (ATG) 3' to the T7 promoter and also the following sequence up to and including the BamH1 restriction endonuclease recognition site:

5'... ATG GGC CAT CAT CAT CAT CAC GGA TCC3' (SEO ID NO.: 3)

5

Sequences inserted into the BamH1 site "in frame" with the initiation codon will therefore be expressed as a fusion protein with the following N-terminal fusion:

(N-terminal) MGHHHHHHHGS.....(C-terminal) (SEQ ID NO.: 4)

10

The fusion of 6 histidines to proteins is commonly used to provide a "tag" for protein purification, usually by affinity for metal ions such as nickel. Since the [T287D] Aurora A sequence coding for amino acids 94-402 was inserted in to the BamHi site, the plasmid encodes for the following protein (using the standard single letter amino acid code):

15

MGHHHHHHGSTQKSKQPLPSAPENNPEEELASKQKNEESKKRQWALEDFEIGRPLGK
GKFGNVYLAREKQSKFILALKVLFKAQLEKAGVEHQLRREVEIQSHLRHPNILRLYGY
FHDATRVYLILEYAPLGTVYRELQKLSKFDEQRTATYITELANALSYCHSKRVIHRDIK
PENLLLGSAGELKIADFGWSVHAPSSRRTDLCGTLDYLPPEMIEGRMHDEKVDLWSL

GVLCYEFLVGKPFFEANTYQETYKRISRVEFIFPDFVTEGARDLISRLLKHNPSQRPML
REVLEHPWITANSSKPSNCONKESASKOS. (SEO ID NO.: 5)

This protein will be referred to in the text as MG-6His-GS-[T287D]Aurora A(94-402).

25 Based on the limited proteolysis studies (described later in Example 1), two additional truncated mutant forms of the Aurora A protein were also generated. The regions encoding for amino acids 113-400 and 122-400 of [T287D]Aurora A were amplified using the polymerase chain reaction (PCR). The 5' PCR primers (5'CATATGCTGGCATCAAAACAGAAAAATG 3' for 113-400 of [T287D]Aurora A or 5'CATATGTCAAAAAAGAGGCAGTGGGC 3' for 122-400 of [T287D]Aurora A) carried a Nde1 restriction endonuclease recognition sequence. A single 3' primer (5'GGATCCTCATTTGCTAGCTGATTCTTTGTTTTGG 3') was used for both constructs and carries a BamH1 recognition sequence and 3' end of the Aurora A sequence following the stop codon. PCR products were purified and cloned into the pCR-

-118-

Script vector (Stratagene) using the pCR-Script AMP cloning kit (Stratagene. product # 211188) according to manufacturers instructions and transfected into the E. coli strain DH5α (Invitrogen product #18258-012). The E. coli colonies containing the recombinant pPCR-Script [T287D]Aurora A(113-400) or pPCRscript [T287D]Aurora A(122-400) were 5 identified by colony PCR screening using the primers T3 (5'AATTAACCCTCACTAAAGGG 3') and T7pro (5'TAATACGACTCACTATAGGG 3') hybridising specifically on either side of the pPCR script vector cloning site. The pPCR-Script vectors carrying the [T287D]Aurora A(113-400) or [T287D]Aurora A(122-400) sequence were prepared from E. coli and were digested with Nde 1 and Bam H1, the digestion products 10 resolved by agarose gel electrophoresis. The fragments containing the [T287D]Aurora A(113-400) or [T287D]Aurora(122-400) were ligated into the expression vector pET28a (Novagen product #69864-3) between the Nde1 and BamH1 restriction sites. The inserted genes were cloned in frame with a sequence coding for a 6 histidine tag followed by a sequence encoding a thrombin protease cleavage site (see below for a complete description). The inserted genes 15 are under the control of a bacteriophage T7 promoter and therefore require expression of the T7 polymerase in trans for efficient transcription in E.coli. The plasmid encodes kanamycin resistance for selection.

The ligation reactions were transfected into DH5α competent E.coli and the bacteria carrying the pET28a-[T287D]Aurora A(113-400) or pET28a-[T287D]Aurora A(122-400)
20 recombinant vectors were identified by their ability to grow on media containing kanamycin.

Plasmid DNAs were extracted from these bacteria and subjected to digestion with the restriction endonucleases Nde1 and BamH1 to identify those carrying the [T287D]Aurora A(113-400) or [T287D]Aurora A(122-400) sequences. The identity of the insert was then confirmed by dideoxy chain termination DNA sequencing prior to protein expression.

pET28a carries the initiation codon (ATG) 3' to the T7 promoter and also the following sequence up to and including the Nde1 restriction endonuclease recognition site:

5'... ATG GGC AGC AGC CAT CAT CAT CAT CAT CAC AGC AGC GGC CTG GTG CCG CGC GGC AGC CAT ATG3'

-119-

Sequences inserted into the Nde1 site "in frame" with the initiation codon will therefore be expressed as a fusion protein with the following N-terminal fusion (using the standard single letter amino acid code):

(N-terminal) MGSSHHHHHHHSSGLVPRGSHM.....(C-terminal)

The fusion of 6 histidines to proteins is commonly used to provide a "tag" for protein purification, usually by affinity for metal ions such as nickel. The motif "LVPRGS" corresponds to a specific thrombin protease cleavage site that allows the proteolytic removal of the sequence "MGSSHHHHHHSSGLVPR" after incubation of the protein with thrombin. Since the [T287D]Aurora A sequences coding for amino acids 113-400 and 122-400 were inserted into the Nde 1 site, the plasmid encodes for the following protein (using the standard single letter amino acid code):

15 [T287D]Aurora A(113-400)

- MGSSHHHHHHSSGLVPRGSHMLASKQKNEESKKRQWALEDFEIGRPLGKGKFGNVY LAREKQSKFILALKVLFKAQLEKAGVEHQLRREVEIQSHLRHPNILRLYGYFHDATRV YLILEYAPLGTVYRELQKLSKFDEQRTATYITELANALSYCHSKRVIHRDIKPENLLLG SAGELKIADFGWSVHAPSSRRTDLCGTLDYLPPEMIEGRMHDEKVDLWSLGVLCYEF
- 20 LVGKPPFEANTYQETYKRISRVEFTFPDFVTEGARDLISRLLKHNPSQRPMLREVLEHP WITANSSKPSNCQNKESASK
 - This protein will be referred to in the text as MGSS-6His-SSGLVPRGSHM-[T287D]Aurora A(113-400)
- 25 [T287D]Aurora A(122-400)
 - MGSSHHHHHHSSGLVPRGSHMSKKRQWALEDFEIGRPLGKGKFGNVYLAREKQSKFI LALKVLFKAQLEKAGVEHQLRREVEIQSHLRHPNILRLYGYFHDATRVYLILEYAPLG TVYRELQKLSKFDEQRTATYITELANALSYCHSKRVIHRDIKPENLLLGSAGELKIADF GWSVHAPSSRRTDLCGTLDYLPPEMIEGRMHDEKVDLWSLGVLCYEFLVGKPPFEAN
- 30 TYQETYKRISRVEFTFPDFVTEGARDLISRLLKHNPSQRPMLREVLEHPWITANSSKPS NCONKESASK
 - This protein will be referred to in the text as MGSS-6His-SSGLVPRGSHM-[T287D]Aurora A(122-400)

Protein expression

pTB375NBSE carrying the [T287D] Aurora A (94-402) sequence were transfected into E.coli BL21(DE3) pLys S (genotype: B F dcm ompT hsdS(r_B⁻ m_B) gal λ(DE3) [pLysS 5 Cam⁵]). The strain was grown for 16 h (LB medium containing tetracycline (10µg/mL) and chloramphenicol (34µg/mL) at 30°C in shake flasks to OD_{550mm} ~5. This culture was inoculated into high biomass medium containing tetracycline (10µg/mL) and chloramphenicol (34µg/mL), in a 20 L fermenter (B. Braun, Melsungen, Germany). Cells were grown aerobically in fed batch culture at 30 °C, pH 6.7 with dissolved oxygen tension maintained at 10 50% air saturation. Expression of 6His-[T287D] Aurora A (94-402) was induced 12 hours post inoculation (OD_{550mm} ~13) with 0.40mM isopropyl-β-D-thiogalactopyranoside (IPTG), and cells harvested 3.0 hours later (OD_{550mm} ~33) by batch centrifugation (7,000xg at 4 °C for 30 min).

pET28a carrying the [T287D]Aurora A(122-400) sequence was transfected into E.coli
DS410 (DE3) (a derivative of the original minicell-producing strain P678-54). The strain was
grown for 30 h (M9 glucose medium containing kanamycin (25μg/mL) at 37°C in shake
flasks to OD_{550mm} ~1.4. This culture was inoculated into high biomass medium containing
kanamycin (25μg/mL) in a 20 L fermenter (B. Braun, Melsungen, Germany). Cells were
grown aerobically in fed batch culture at 30°C, pH 6.7 with dissolved oxygen tension
maintained at 50% air saturation. Expression of MGSS-6His-SSGLVPRGSHM[T287D]Aurora A(122-400) was induced 16 hours post inoculation (OD_{550mm} ~19) with
0.10mM isopropyl-β-D-thiogalactopyranoside (IPTG), and cells harvested 23 hours later
(OD_{550mm} ~26) by batch centrifugation (7,000xg at 4°C for 30 min).

Definition of kinase domain fragment

25

MG-6His-GS-[T287D]Aurora A(94-402) was purified from E. coli cell paste by NiNTA Agarose chromatography followed by size exclusion chromatography. The solution
properties of this protein were found to be unfavourable for structural studies. Limited
proteolysis of MG-6His-GS-[T287D]Aurora A(94-402) was used to identify fragments of the
Aurora A kinase domain with superior solution properties. Aliquots of MG-6His-GS[T287D]Aurora A(94-402) were subjected to proteolytic digestion with trypsin, thermolysin

-121-

or endoproteinase Glu-C (V8). Protein fragments were identified by analysis with Coomassiestained SDS PAGE, electrospray mass spectrometry (ESMS) and N-terminal sequencing.

Cleavage and purification was performed at sufficient scale to produce appropriate quantities of [T287D]Aurora A (122-396) for crystallisation, as detailed below. Characterization of these fragments of Aurora A was used to design additional constructs, including MGSS-6His-SSGLVPRGSHM-[T287D]Aurora-A(122-400). The molecular biology procedures used to generate MGSS-6His-SSGLVPRGSHM-[T287D]Aurora-A(122-400) are given in the Molecular Biology section of Example 1.

10 Lysis of E. coli containing MG-6His-GS-[T287D]Aurora A(94-402)

The following procedures were performed at 4°C unless otherwise stated.

E. coli cell paste (200 g) was resuspended using a Kinematica PT6000 homogeniser
(Kinematica GMBH, Basel, Switzerland) in 1.0 l of lysis buffer (40mM HEPES, 200mM
NaCl, 2mM imidazole, 2mM 2-mercaptoethanol, 1mM benzamidine, pH 7.4). The cells were
lysed using an Avestin EmulsiFlex fiC5 (Avestin, Inc., Ottawa, Canada), using a single pass at
an average pressure of 10,000 psi. The resulting lysate was centrifuged at 17,000 x g (average)
for 90 min before aspirating the supernatant and discarding the pellet.

Lysis of E. coli containing MG-6His-GS-[T287D]Aurora A(94-402)

The following procedures were performed at 4 °C unless otherwise stated.

E. coli cell paste (200 g) was resuspended using a Kinematica PT6000 homogeniser
(Kinematica GMBH, Basel, Switzerland) in 1.0 l of lysis buffer (40mM HEPES, 200mM
NaCl, 2mM imidazole, 2mM 2-mercaptoethanol, 1mM benzamidine, pH 7.4). The cells were
lysed using an Avestin EmulsiFlex ñC5 (Avestin, Inc., Ottawa, Canada), using a single pass at
an average pressure of 10,000 psi. The resulting lysate was centrifuged at 17,000 x g (average)
for 90 min before aspirating the supernatant and discarding the pellet.

Preparation of [T287D]Aurora A(122-396)

The following procedures were performed at 4°C unless otherwise stated.

30 A 26 mm diameter chromatography column packed with 25 mL Qiagen Ni NTA-Agarose (Qiagen GMBH, Hilden, Germany) was equilibrated with 10 column volumes of lysis buffer before loading lysate supernatant containing MG-6His-GS-[T287D]Aurora A(94-402) onto

-122-

the column at a flow rate of 0.9 mL/min. Using a flow rate of 2.0 mL/min the column was washed with 10 column volumes of wash buffer (40mM HEPES, 20mM imidazole, 2mM 2mercaptoethanol, pH 7.5) to remove weakly bound or non-specifically bound impurities. Elution of bound protein was effected using elution buffer (40mM HEPES, 400mM 5 imidazole, 2mM 2-mercaptoethanol, pH 7.5) at 2.0 mL/min. Eluted material was flowed through a second chromatography column (26 mm diameter, packed with 25 mL Pharmacia Q Sepharose Fast Flow (Amersham Pharmacia Biotech, Uppsala, Sweden) previously equilibrated with 10 column volumes of wash buffer). Fractions of 10.0 mL were collected, and after analysis by Coomassie-stained SDS PAGE, those fractions containing significant 10 amounts of MG-6His-GS-[T287D]Aurora A(94-402) were pooled. At this stage the pool (approximately 200 mL) was stored in an airtight container at 4 °C for up to seven days.

From this stage forward, all procedures were carried out at room temperature, unless otherwise stated. A Pharmacia HiPrep 16/60 Sephacryl S-100 pre-packed size exclusion column was equilibrated in running buffer (40 mM HEPES pH7.5, 350 mM NaCl, 2 mM 15 dithiothreitol (DTT)). The column was run at a flowrate of 1.0 mL/min. A 10 mL sample of the MG-6His-GS-IT287D1Aurora A(94-402) pool was centrifuged (31,000 x g, 4 °C, 60 min) and loaded onto the column. The fractions (2.0 mL) were analysed by Coomassie-stained SDS PAGE, and those containing MG-6His-GS-[T287D]Aurora A(94-402) were pooled.

Limited proteolysis at room temperature was carried out on the size exclusion 20 chromatography-purified pool of MG-6His-GS-[T287D]Aurora A(94-402), whose concentration was 1 mg/mL. Using a mass ratio of 1 part protease to 100 parts MG-6His-GS-[T287D]Aurora A(94-402), endoproteinase Glu-C from Staphylococcus aureus V8 (Boehringer Mannheim UK, Lewes, Sussex, UK) was added to the pool. Proteolysis was allowed to continue for between 3 and 7 h.

25

A chromatography column was packed with a mixture of Pharmacia Sephacryl S-100 HR and Pharmacia Q-Sepharose high performance in the ratio of 9:1 v/v respectively (referred to as 'the S-100/Q column'). The column volume was 130 mL. It was equilibrated and run in S-100/Q running buffer (40 mM HEPES pH7.5, 50 mM NaCl, 2 mM dithiothreitol) at a flowrate of 1.0 mL/min. A sample of the proteolysed pool (8 mL) was loaded onto the S-30 100/Q column and 2.0 mL fractions were collected. Fractions were analysed by Coomassiestained SDS PAGE, and those containing significant quantities of pure [T287D]Aurora A(122-396) were pooled. A sample of the pool was analysed by LC-ESMS using a Micromass

-123-

LCT in conjunction with a Waters Alliance HPLC (Micromass, Manchester, UK). A further sample of the pool was subjected to N-terminal sequencing. Once the identity of the cleaved protein had been confirmed as [T287D]Aurora A(122-396), it was submitted for crystallisation.

5

Preparation of GSHM-[T287D]Aurora A(122-400)

The following procedures were performed at 4°C unless otherwise stated.

A 26 mm diameter chromatography column packed with 15 mL Qiagen Ni NTA-Agarose (Qiagen GMBH, Hilden, Germany) was equilibrated with 10 column volumes of lysis buffer
before loading lysate supernatant containing MGSS-6His-SSGLVPRGSHM-[T287D]AuroraA(122-400) onto the column at a flow rate of 1.0 mL/min. Using a flow rate of 2.0 mL/min
the column was washed with 7 column volumes of wash buffer (40mM HEPES, 200mM
NaCl, 10mM MgCl₂, 20mM imidazole, 2mM 2-mercaptoethanol, pH 7.5) to remove weakly
bound or non-specifically bound impurities. Elution of bound protein was effected using
elution buffer (40mM HEPES, 400mM imidazole, 10mM MgCl₂, 2mM 2-mercaptoethanol,
pH 7.5) at 2.0 mL/min. Fractions of 10.0 mL were collected, and after analysis by Coomassiestained SDS PAGE, those fractions containing significant amounts of MGSS-6HisSSGLVPRGSHM-[T287D]Aurora-A(122-400) were pooled.

From this stage in the purification onward, all procedures were carried out at room
temperature unless otherwise stated. A Pharmacia HiPrep 26/10 Fast Desalting pre-packed
column was equilibrated in running buffer (40 mM HEPES pH7.4, 150 mM NaCl, 2 mM 2mercaptoethanol). The column was run at a flowrate of 3.0 mL/min. A 10 mL sample of the
MGSS-6His-SSGLVPRGSHM-[T287D]Aurora-A(122-400) pool was filtered (0.22µm) and
loaded onto the column. Fractions were collected, and those containing the most concentrated
amounts of MGSS-6His-SSGLVPRGSHM-[T287D]Aurora-A(122-400) were pooled.

Bovine thrombin (500 units, Amersham Pharmacia Biotech) was added to the pool of 50 mg (4/- 20%) of purified MGSS-6His-SSGLVPRGSHM-[T287D]Aurora-A(122-400) whose concentration was 1 mg/mL. Specific proteolytic cleavage was allowed to proceed to completion at 4°C, producing the truncated mutant GSHM-[T287D]Aurora A(122-400).

A Pharmacia HiPrep 16/60 Sephacryl S-100 pre-packed size exclusion column was equilibrated in running buffer (40 mM HEPES pH7.4, 50 mM NaCl, 1 mM dithiothreitol). The column was run at a flowrate of 1.0 mL/min. A 10 mL sample of the GSHM-

-124-

[T287D]Aurora A(122-400) pool was filtered (0.22µm) and loaded onto the column.

Fractions (2.0 mL) were analysed by Coomassie-stained SDS PAGE, and those containing GSHM-[T287D]Aurora A(122-400) were pooled, and submitted for crystallisation.

5 Analysis

For SDS PAGE all samples were diluted in Laemmli buffer containing 2-mercaptoethanol, boiled for 2 minutes and loaded onto a 8-16% gradient, 1.5mm thickness x 10 well NOVEX gel (NOVEX, San Diego, California). Gels were stained with Coomassie blue R-250. Edman degradation was carried out on a Perkin Elmer 477A peptide sequencer (Applied Biosystems, 10 Foster City, CA) with on-line detection of PTH amino acids. Mass spectra were acquired using a Micromass LCT with electrospray source (Micromass, Manchester, UK) and on-line Waters 2790 Alliance delivery system (Waters, Milford, MA). Protein was loaded directly on to a Phenomenex Jupiter 5μ C5 300_ 150 x 2.00 mm reverse phase column equilibrated in Milli Q water (Millipore, Bedford, MA), 2.7% acetonitrile, 0.1% trifluoroacetic acid, and the 15 column was developed with a 2.7% to 90% acetonitrile gradient over 30 minutes at a flowrate of 80μl/min. A fraction (approximately 25%) of the eluted proteins passed into the mass spectrometer.

20 Example 2: Crystallisation of [T287D] Aurora A catalytic domain constructs

The [T287D] Aurora A(122-396):AMPPNP complex was crystallized at 15°C by the method of hanging-drop vapour diffusion. The protein [T287D] Aurora A (122-396) was concentrated to -10 mg/ml. solution (in 40mM HEPES pH 7.4, 2mM DTT, 50mM NaCl), 25 5mM AMP-PNP was then added to this solution and the complex was incubated on ice for 30 minutes. Prior to setting up crystallization trials this complex solution was microfuged for 10 minutes. The drops contained a 1:1 by volume mixture of complex solution and reservoir buffer (0.2M K₂HPO₄, 1.6M NaH₂PO₄, 0.1M phosphate/citrate buffer pH 3.8) giving a final 4μl drop volume. The [T287D] Aurora(122-396)-AMP-PNP crystals belong to space group 30 P3₂21 with unit cell dimensions a = b = 86.55 Å, c = 78.34 Å, and æβ=90°, γ=120°, and contain 1 complex molecule per asymmetric unit. Before data collection, the crystals were transferred briefly (for about 20 seconds) to a cryobuffer containing 0.2M K₂HPO₄, 1.6M

-125-

 ${
m NaH_2PO_4}$, 0.1M phosphate citrate pH 3.8, 30% glycerol before being cooled to 100K in a nitrogen gas stream.

The GSHM-[T287D] Aurora A(122-400) complex with the chemically synthesized inhibitor of formula II was crystallized as follows. Preparation of compound of formula II is 5 described under example 19 in patent publication number WO 01/21597, publication date 29/3/01 (application number PCT/GB00/03593, international filing date 19/09/00). The compound was added at 5mM to a solution containing protein (GSHM-[T287D] Aurora A(122-400) at 10mg/ml, 40mM HEPES pH7.5, 50mM NaCl, and 1mM 2-mercaptoethanol. Drops were formed by mixing 1:1 volumes of protein complex solution and a reservoir solution containing 22% PEG 4000 and 0.2M ammonium sulphate. Crystallisation was achieved by hanging drop vapour diffusion at 15°C. Data were collected at room temperature from a crystal mounted in a capillary. The crystal could be translated in the X-ray beam to allow multiple exposures. The Aurora A-inhibitor crystals are of space group P2₁ with unit cell dimensions a = 52.6, b = 88.4, c = 67.8 Å, $\alpha = \gamma = 90$ and $\beta = 90.01^\circ$, and contain two

Example 3: Structure determination of [T287D] Aurora A catalytic constructs

Diffraction data were collected at beamline PX9.6 at the SRS, Daresbury on an ADSC

Quantum 4 CCD detector. The data were indexed and integrated with the program Mosflm
and scaled with the program SCALA (CCP4). Molecular replacement and rigid body
refinement to a resolution of 3.0 Å were carried out using the program AMoRe. A search
model was derived from mouse PKA, truncating the model at residues 32 to 310 and replacing
all non-identical residues with Ala. 5% of the data were reserved at this stage as a crossvalidation set and the initial model underwent torsion angle simulated annealing in the
program CNX using a maximum likelihood target and an overall anisotropic temperature
factor correction. The model then underwent iterative rounds of manual rebuilding and
simulated annealing until the working R-factor fell below 30%, at which point restrained
isotropic individual temperature factor refinement was carried out. Concurrent building of
both inhibitor complexes with the same Aurora protein in different crystal forms proved very
instructive when it came to clarification of regions that were difficult to interpret. Further
iterative rebuilding and addition of waters was carried out until the free R factor converged.

Crystallographic data and refinement statistics are given in tables 4 and 5.

Table 4: Aurora-AMPPNP complex data and refinement statistics.

Space Group	P3 ₂ 21
Cell constants	a=b=86.55, c= 78.34Å α=β=90, γ=120°
Reflections	62278
Independent Reflections	17003
R _{sym} (2.25-2.2 Å)	3.6% (32.6%)
Resolution (Å)	38-2.2
I/sigI (2.25-2.2 Å)	19.3 (3.0)
Completeness (2.25-2.2 Å)	97.1% (83.2%)
R _(free) , R _(work)	23%, 28%
Rmsd (bond lengths)	0.006
Rmsd (bond angles)	1.2

Table 5: Aurora-inhibitor complex data and refinement statistics:

Space Group	P2 ₁
Cell constants	a=52.6, b=88.4, c=67.8Å α=γ=90, β=90.01°
Reflections	36664
Independent Reflections	26294
R _{sym} (2.25-2.1 Å)	6.6% (30.5%)
Resolution (Å)	52-2.1
I/sigI (2.25-2.1 Å)	7 (2.1)
Completeness (2.25-2.1 Å)	72.5% (25.5%)
R _(free) , R _(work)	22%, 27%
Rmsd (bond lengths)	0.019
Rmsd (bond angles)	1.8

Example 4: Description of the Structure of Aurora A kinase

5

The structure of [T287D] Aurora A (122-396) in a binary complex with the ATP analogue AMP-PNP has been solved to a resolution of 2.2 Å. The structure of GSHM-[T287D] Aurora A(122-400) in a binary complex with the synthetic inhibitor of formula II has been solved to a resolution of 2.1 Å. The structures contain the residues of the kinase catalytic domain. The kinase domain of [T287D] Aurora A shows the bilobal structure 10 characteristic of protein kinases with the ATP and inhibitor binding site situated between the two lobes. The N-terminal domain (lobe) comprises a twisted β-sheet and a single kinked helix. The C-terminal lobe comprises mainly helices but also includes a small region of \betasheet. Parts of the polypeptide chain are disordered. In particular, the activation loop, residues 279 to 290 containing the T287D substitution, is not visible in the electron density. 15 The disordered nature of the activation loop is a common feature in kinase crystal structures.

The structure adopts a conformation typical of catalytically inactive kinases, despite the introduction of the constitutively active mutation, T287D. It is thought that the acidic pH at which the crystallisation experiments were carried out will result in the introduced aspartate being protonated, and thus no longer able to mimic the phosphorylated threonine in the wild-20 type activated protein. The kinase activity of the mutant enzyme towards a peptide substrate was measured at varying pH values, as shown in Figure 3, and indeed, activity is significantly reduced falls as the pH is lowered.

The inactive conformation seen in our [T287D] Aurora A complexes is clearly capable of binding the inhibitor of formula II and the ATP analogue, and therefore allows structure-25 based design, which needs to make allowances for the flexibility and conformational changes that the kinase may undergo, for example, between its active and inactive states. In the case of the inhibitor, the inactive conformation may be forced by the steric bulk of the inhibitor.

Aurora A is quite closely related to the cyclic AMP-dependent protein kinase, also known as PKA, and the structures superpose with an overall rmsd of 1.4Å. The ATP binding 30 cleft of Aurora A is more extended than the equivalent cleft in PKA on account of a shift in the position of a helix, formed by residues 174 to 182 in the N-terminal lobe. In the structure of [T287D] Aurora A, the helix is displaced approximately 3Å away from the ATP binding pocket compared with the equivalent helix in PKA, thus extending the length of the cleft

-128-

between the two lobes. The extended cleft can be exploited by elongated inhibitor molecules such as that of formula II and may be key to the design of specific inhibitors. The conserved DFG motif (Asp273Phe274Glu275) preceding the activation loop is apparent in the electron density. This region contains an aspartate residue necessary for catalysis. The glycine-rich loop, which is important for ATP binding in all kinases, shows good electron density throughout the main chain atoms, although the temperature factors are quite high, indicating significant mobility of the loop. However, the density for the side chains of some residues, such as Phe 143, is poor, and these are likely to adopt multiple conformations.

The AMP-PNP molecule adopts a dual conformation (Fig. 1). The adenine ring and ribose moiety in both conformations occupy similar locations with respect to the kinase molecule. Classical hydrogen-bonding interactions are made between the adenine ring and the hinge region of Aurora A. These are between N6 of the adenine ring and the main chain oxygen of Glu 210 and between N1 of the adenine ring and the main chain nitrogen of Ala 212. The differences in the two conformations arise from torsion angle differences between 15 the ribose ring and the phosphate groups and also in torsion angles of phosphorus-oxygen bonds. In one conformation, the β-phosphate group forms a hydrogen bond to a water molecule, which, in turn, forms a hydrogen bond to Asp 273. In the other conformation, the β-phosphate forms hydrogen bonds with Ser 277 and Gln 260. In both conformations the α-phosphate forms a salt-bridge with Lys 161, and also forms a hydrogen bond with the main 20 chain nitrogen of Val 278. No electron density for the γ-phosphate is present in either conformation suggesting a high degree of disorder. This disorder of the γ-phosphate has also been seen in other crystal structures, for example that of Checkpoint kinase.

The molecule of formula II also binds in the ATP binding site in the cleft between the two domains in the Aurora A kinase molecule. The molecule of formula II adopts an extended conformation, which demonstrates the extent of the available binding pocket (Fig 2b). A classical kinase (adenine-mimetic) inhibitor hydrogen bond interaction with the main chain peptides is made between N(17) in the inhibitor and the amide of amino acid residue 212. The piperidine moiety of the inhibitor extends into solvent (on the left in Fig 2b). At the other extreme of the inhibitor (right end in Fig 2b) the benzoyl moiety fits into a hydrophobic pocket formed by residues Leu163, Leu181, Leu195, Leu207 and Trp276. This inhibitor represents a more interesting start point for design than AMPPNP since protein regions more remote from the ATP location are explored, and this may help achieve specificity.

-129-

CLAIMS

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What we claim is:

- 5 1. A crystalline form of a polypeptide comprising the catalytic domain of Aurora kinase.
 - A crystalline form according to Claim 1, wherein the polypeptide is an Aurora A kinase
- 10 3. A crystalline form according to Claim 1 or Claim 2, wherein the crystalline form has the space group P3₂21 or the space group P2.
- A crystalline form according to any one of the preceding claims, wherein the
 crystalline form has unit cell dimensions a=b=86.55, c= 78.34 Å, α=β=90 and γ=120° or unit
 cell dimensions a = 52.6, b = 88.4, c = 67.8 Å, α=γ = 90 and β= 90.01°.
- 5. A crystalline form according to any one of the preceding claims, wherein the catalytic domain comprises a binding site, wherein the binding site is defined by the x,y,z-coordinates of atoms in the set of amino acid residues given by the list: Arg136, Leu138, G1y139, Lys140, 20 Gly141, Val146, Ala159, Lys161, Leu163, Va1177, Glu180, Val181, Ile183, G1n184, Leu193, Leu195, Leu207, Leu209, G1u210, Tyr211, Ala212, Pro213, Leu214, G1y215, Thr216, Arg219, G1u259, Asn260, Leu262, Ala272, Asp273, Phe274, Gly275, Trp276, Ser277, Va1278, and His279 or their equivalent, wherein the atomic coordinates are listed in Tables 1 and 2; or wherein the binding site is defined by the x,y,z-co-ordinates of atoms in the set of amino acid residues given by the list: Arg136, Leu138, Gly139, Va1146, Ala159, Lys161, Leu163, Ile183, G1n184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215, Thr216, Arg219, Glu259, Asn260 and Leu262 or their equivalent, and wherein the x,y,z-coordinates are within a root mean square deviation of not more than 1.0 Å of the coordinates listed in Tables 1 and 2.
 - A crystalline form according to any one of the preceding claims, additionally comprising an Aurora kinase inhibitor in complex with the catalytic domain of Aurora kinase.

-130-

 A crystalline form according to Claim 6, wherein the Aurora kinase inhibitor is a compound of formula II:

Formula II.

- 5
 - A method of designing an Aurora chemical modulator using the atomic coordinates of a crystalline form according to any one of claims 1 to 5.
- A method of selecting an Aurora chemical modulator using the atomic coordinates of a
 crystalline form according to any one of claims 1 to 5.
 - A method of designing an Aurora protein using the atomic coordinates of a crystalline form according to any one of claims 1 to 5.
- 15 11. A method of designing or selecting an Aurora modulator comprising the steps of: (a) exploring the atomic coordinates of Aurora as presented in Table 1 and Table 2 for information on the three-dimensional characteristics of the protein surface; (b) arriving at an alternative overlapping or non-overlapping binding pocket to the active site ATP binding pocket; and (c) selecting or designing an Aurora modulator using the binding pocket information.
- 12. A method of designing the three-dimensional structure of a second crystal form of Aurora kinase comprising the step of applying difference Fourier or molecular replacement methods using the atomic coordinates of an original crystal as presented in Table 1 and Table 2 to model the structure of the crystal second form, wherein the active site ATP binding pocket of the second crystal form is equivalent to that in the original crystal.

-131-

- 13. A method of designing or selecting an Aurora kinase modulator using the coordinates of any protein shown by this invention to possess structural similarity or relevance to Aurora kinase.
- 5 14. A method for designing a homologue of Aurora kinase that mimics the threedimensional structure of Aurora kinase, which comprises:

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- (i) determining the three-dimensional coordinates of atoms of an Aurora kinase;
- (ii) providing a computer having a memory means, a data input means, a visual display means, said memory means containing three-dimensional molecular simulation software operable to retrieve co-ordinate data from said memory means and to display a three-dimensional representation of a molecule on said visual display means and being operable to produce a modified three-dimensional homologue representation responsive to operator-selected changes to the structure of the Aurora kinase and to display the three-dimensional representation of the modified three-dimensional homologue;
- iii) inputting three-dimensional co-ordinate data of atoms of Aurora kinase into the computer and storing said data in the memory means;
- inputting into the data input means of said computer at least one operatorselected change in structure of the Aurora kinase;
- (v) executing said molecular simulation software to produce a modified threedimensional molecular representation of the homologue structure;
 - (vi) displaying the three-dimensional representation of the homologue on said visual display means, whereby changes in three-dimensional structure of the Aurora kinase resulting from changes on structure can be visually monitored;
- (vii) repeating steps (iv) through (vi) to produce a multiplicity of homologues;
 - (ix) selecting a homologue structure represented by a three-dimensional representation wherein the three-dimensional configuration and spatial arrangements of the kinase catalytic domain remain substantially preserved, thereby producing a homologue of Aurora kinase that mimics the threedimensional structure of the Aurora kinase.
- 15. A method of producing a modulator of Aurora kinase comprising identifying a compound or molecule or designing a compound or molecule that fits into the active site ATP

-132-

binding pocket of the Aurora kinase, wherein the ATP binding pocket is defined by the x,y,z-coordinates of atoms in the set of amino acid residues given by the list (a) Arg136, Leu138, Gly139, Lys140, Gly141, Val146, Lys161, Leu163, Val177, Glu180, Val181, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215,

- 5 Thr216, Arg219, Glu259, Asn260, Leu262, Ala272, Asp273, Phe274, Gly275, Trp276, Ser277, Val278, and His279, the atomic coordinates being listed in Tables 1 and 2 or (b) the x,y,z- coordinates of atoms in the set of amino acid residues given by the list Arg136, Leu138, Gly139, Val146, Ala159, Lys161, Leu163, Ile183, Gln184, Leu193, Leu195, Leu207, Leu209, Glu210, Tyr211, Ala212, Pro213, Leu214, Gly215, Thr216, Arg219, Glu259, Asn260 and
- 10 Leu262, each having coordinates as described in Tables 1 and 2, thereby producing a modulator of Aurora kinase.
- A crystalline form wherein the catalytic domain comprises a binding site , wherein the binding site is defined by the x,y,z-co-ordinates of atoms in the set of amino acid residues
 given by the list: Leu138, Gly139, Val146, Lys161, Val177, Arg178, Arg179, Glu180, Val181, Glu182, Ile183, Gln184, Leu193, Leu209, Tyr211, Ala212, Gly215, Thr216, Glu259, Asn260, Leu262, Ala272, Asp273, Phe274, Gly275, Trp276, Ser277, Val278 and His279 or their equivalent, wherein the atomic co-ordinates are listed in Table 1a.

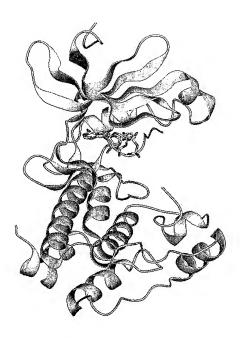


Figure 1

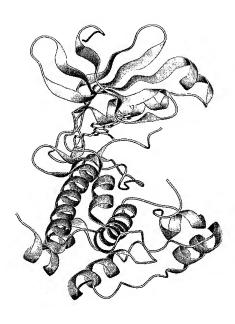


Figure 2a

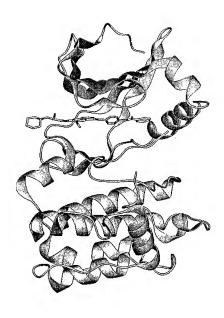


Figure 2b

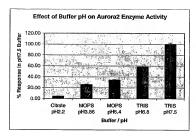


Figure 3